A critical analysis of emission quantification methods in the ferrochrome industry

K Campbell

orcid.org/0000-0002-0670-045X

Thesis submitted in fulfilment of the requirements for the degree *Doctor of Philosophy in Mechanical Engineering* at the North-West University

Promoter: Prof M Kleingeld

Graduation ceremony: May 2019

Student number: 22171444

Acknowledgements

Hereby, the author would like to show her gratitude by thanking persons that have had any influence on the completion of this research study:

- Thanks to Prof E.H. Mathews and Prof M. Kleingeld for giving me the opportunity to continue with my post-graduate studies and development as an engineer.

- To my study leader, Prof M. Kleingeld, and my colleagues at ETA Operations (Pty) Ltd who made this thesis possible. Thank you for the support and assistance. None of this would be possible without you.

- To Dr Walter Booysen, thank you for the assistance, support and leadership with this thesis. Thank you for being the best mentor and always being prepared to help. Your dedication is truly appreciated.

- To my sister (Karin), brother-in-law (Nicohan) and all of my friends, for all their love and support during the completion of this research study.

- To, my parents, Quentin and Erika Campbell. Thank you for your love. I am very grateful to have parents that have sacrificed so much for me. You are a great example to me.

- A very special thanks to my husband, Diaan Nell, for all your love and support throughout this time. Your support is highly appreciated, and I love you very much.

- Finally, I would like to thank God for His grace and unconditional love. Without Him, none of this would be possible.

Abstract

Title: A critical analysis of emission quantification methods in the ferrochrome industry

Author: K. Campbell

Promoter: Prof M. Kleingeld

Keywords: *CO_2 emissions, ferrochrome industry, carbon tax, mass balance, critical analysis*.

Ferrochrome (FeCr) furnaces are significant CO_2 emitters due to the large amounts of carbon-containing materials being used. FeCr industries will therefore become liable for carbon tax (CT), which is set for implementation in 2019. To estimate the CT liability of a certain entity, the CO_2 emissions must be determined as accurately as possible. However, the prescribed way to quantify these emissions is overly generic and the implementation thereof still uncertain. This study was therefore conducted to critically assess the CO_2 emission quantification methods available to the FeCr industry.

Unfortunately, the initial research showed that there are no detailed analyses or practical examples available. The lack of detail and case studies limits insights available on the practical and operational reality and how it can affect the results produced by the prescribed methods. It was therefore necessary to perform a critical literature analysis of the emission quantification methods to determine the associated risks for the ferrochrome industry. This comprehensive analysis, using a significant amount of literature references, aimed to identify the main focus areas of the study.

The focus areas identified are (1) practical application of prescribed methods, (2) refinement of the prescribed methods and (3) comparison of the different methods. Three separate chapters are dedicated to develop and verify methodologies for each focus area. The verifications were done using practical case studies from 17 different FeCr furnaces, all situated in South Africa.

Focus area 1: Although there are prescribed methods (tier 1, 2 and 3) to perform the emission calculation of a FeCr furnace, there was a lack of literature studying the practical application, as well as the implications associated with these methods. The three prescribed calculation methods were therefore evaluated and applied to 17 case studies. It was found that one is likely to obtain results with errors ranging from 8.9% - 18.8% when performing the prescribed calculations.

Focus area 2: The prescribed calculation methods are relatively simple to apply but produce results with varying levels of accuracy. The need was therefore established to refine these prescribed methods to improve the accuracy of the results. The developed methodology delivered a systematic approach to refine the prescribed tier 3 mass balance approach. The case studies proved that by constructing an *advanced mass balance*, a much smaller error (2.4%) will be achieved, adding to the reliability of the final results.

Focus area 3: The study presented six quantification methods (three prescribed and three developed methods) and applied all the methods to 17 case studies. A comparison of the generated results shows a variance of 13-33% on the calculated CO_2 emission result. This translates to a variance of R75 million – R185 million per year in carbon tax liability. An evaluation of the associated accuracies also shows a wide range of variance from tier 1 (25%-50% error) to tier 3 (<5% error).

The complexity of the different methods increases significantly between the prescribed methods and the refined mass balances. It was found, however, that with a little extra "complexity" a much higher accuracy can be accomplished. Based on the method developed throughout this study, and based on the case studies performed, the advanced mass balance gives an average error of 2.4%.

A significant contribution of the approach is realised by improved CT liability estimation. The monetary value for the entire FeCr industry in SA has decreased throughout the course of this study. From an initial estimation of R562 million per annum with a 50% uncertainty (purely based on literature assumptions) to a value of R448 million with a 2.4% uncertainty (based on the use of methods developed within this study). The developed approach is therefore confirmed to make a critical contribution to the emission quantification methods for FeCr furnaces.

Table of contents

List of figures

List of tables

List of equations

List of abbreviations

Abbreviation	*Description*
AC	Alternating current
B	Book
BF	Blast furnace
BOF	Basic oxygen furnace
C	Composition
CP	Conference paper
CS	Case study
CT	Carbon tax
DC	Direct current
e.g.	Example
EF	Emission factor
et al.	And others
F1, 2 …	Furnace 1, 2 …
GHG	Greenhouse gases
i.e.	That is
IPCC	Intergovernmental Panel on Climate Change
JA	Journal article
kWh	Kilowatt hours
M	Mass
MB1, 2, 3	Mass balance 1, 2, 3
Mt	Megatonne
N/OD	National or official documentation

Prox	Proximate analysis
PSP	Pelletising and sintering plant
R	Report
SA	South Africa
t	Tonne
T/D	Thesis or dissertation
T1, 2, 3	Tier 1, 2, 3
TCM	Training course material
TEC	Total elemental composition
Ult	Ultimate analysis
ZAR	South African Rand

Chemical elements and compounds

Al	Aluminium
C	Carbon
Ca	Calcium
Cr	Chromium
H	Hydrogen
Mg	Magnesium
N	Nitrogen
O	Oxygen
S	Sulphur
Si	Silicon
Al_2O_3	Aluminium oxide
$CaCO_3$	Calcium carbonate
$CaMg(CO_3)_2$	Calcium magnesium carbonate

CaO	Calcium oxide
CH_4	Methane
CO	Carbon monoxide
CO_2	Carbon dioxide
Cr_2O_3	Chromium(III) oxide
Fe_2O_3	Iron(III) oxide
$FeCr$	Iron(II) chromite (*Ferrochrome*)
$FeMn$	Ferromanganese
$FeMo$	Ferromolybdenum
FeO	Iron(I) oxide
$FeSi$	Ferrosilicon
FeV	Ferrovanadium
FeW	Ferrotungsten
H_2	Hydrogen
H_2O	Water
K_2O	Potassium oxide
MgO	Magnesium oxide
N_2	Nitrogen
N_2O	Dinitrogen monoxide
Na_2O	Sodium oxide
NO	Nitrogen oxide
P_2O_5	Phosphorus pentoxide
SiO_2	Silicon dioxide
SO_3	Sulphur trioxide
TiO_2	Titanium dioxide

List of symbols

Symbol	***Description***
μ	Mean / average
σ	Standard deviation
%	Percentage
E_{CO_2}	CO_2 emissions from ferroalloy production
MPi	Production of ferroalloy type *i*
EFi	Generic emission factor for ferroalloy type *i*
$M_{reducing\ agent,\ i}$	Mass of reducing agent *i*
$EF_{reducing\ agent,\ i}$	Emission factor of reducing agent *i*
$CContent_{reducing\ agent,\ i}$	Carbon (C) content in reducing agent *i*
$M_{ore,\ h}$	Mass of ore *h*
$CContent_{ore,\ h}$	C content in ore *h*
$M_{slag\text{-}forming\ material,\ j}$	Mass of slag-forming material *j*
$CContent_{slag\text{-}forming\ material,\ j}$	C content in slag-forming material *j*
$M_{product,\ k}$	Mass of product *k*
$CContent_{product,\ k}$	C content in product *k*
$M_{non\text{-}product\ outgoing\ stream,\ l}$	Mass of non-product outgoing stream *l*
$CContent_{non\text{-}product\ outgoing\ stream,\ l}$	C content in non-product outgoing stream *l*

1. GENERAL INTRODUCTION

1.1. Background

Ferrochrome production

The process of ferrochromium (FeCr) production is an energy-intensive one [1, 2, 3]. The total electricity consumption of such a process typically ranges between 3.3 and 4.2 kWh/t of FeCr produced [4, 5, 6, 7, 8]. FeCr is mainly used for stainless steel production, where approximately 1 tonne is needed to produce 3 – 3.5 tonnes of stainless steel [9].

Production is accomplished by feeding raw materials in the form of chromite ores, carbon-rich materials (reductant), and additives (fluxes, in the form of quartz, limestone, dolomite, etc.) to an arc furnace [10, 11]. Electricity is used to heat up the furnace and melt the raw materials by means of an electric arc [12].

Various chemical reactions take place, with the main objective to reduce the metal oxides in the chromite ore to a final metal product, ferrochromium. Together with the main metal product, waste material (slag), as well as off-gas, also exit the furnace as by-products [13]. The diagram below shows a simplified illustration of this process.

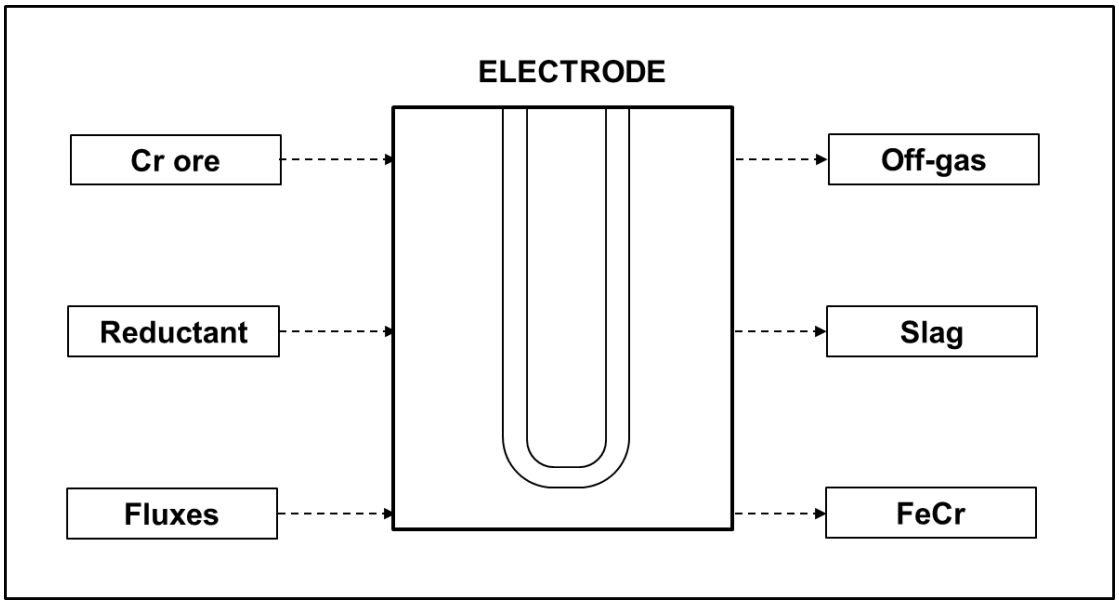


Figure 1-1: Overview of the FeCr production process

Emissions from FeCr production

According to Niemelä [14], the process of FeCr production generates a significant amount of off-gas, mainly in the form of carbon emissions, including carbon monoxide (CO) and carbon dioxide (CO_2). The following table shows common off-gas compositions of a typical FeCr furnace.

Table 1-1: Typical off-gas composition for a FeCr furnace (volumetric percentage)

Component	**Niemelä *et al.*** [14] **Beukes *et al.*** [15]	**Du Preez** [11]	**Riekkola-Vanhanen** [3] **Kapure *et al.*** [13]
CO	75 - 90	60 - 90	85 - 90
CO_2	2 - 10	10 - 40	2 - 5
H_2	2 - 15	2 - 10	5 - 7
N_2	2 - 7	2 - 10	2 - 5

From the table, Niemelä's statement is supported, as the majority of the off-gas consists of carbon emissions. The off-gas from a closed furnace (consisting mainly of CO) can either be utilised for bio-ethanol or energy production, or be flared (converts to CO_2) [16]. In open or semi-closed furnaces, the CO produced is burnt within the furnace, above the charge level, to CO_2. It is assumed that all CO gas emitted to the atmosphere eventually converts to CO_2 [16]. The National Inventory Report of Norway confirms that the production of FeCr only generates CO_2 emissions, when considering the official greenhouse gas (GHG) emissions only: CO_2, CH_4 and N_2O [17, 18].

Carbon tax and FeCr in South Africa

The South African Department of Environmental Affairs [19] lists fifteen processes which represent the majority of the industrial sectors in South Africa (SA). Amongst these, the production of ferroalloys is included. Entities on this list must submit a pollution prevention plan to the Minister, and can be considered as future carbon tax payers [20].

To adhere to the commitment made in lowering the national GHG emissions [21], carbon tax is proposed to be introduced in SA soon [22]. According to the February 2018 budget speech [23], the original date of implementation is 1 January 2019. However, this date will be postponed to 1 June 2019, according to the Medium Term Budget Policy Statement (October 2018) [24].

The main goal of carbon tax is to reduce the total national GHG emissions in South Africa. Official carbon tax documentation states that all industries emitting more than 0.1 Mt of GHG emissions (FeCr industries unfortunately qualifying) must submit a pollution prevention plan to the Minister, and will also be liable to pay carbon tax [20]. The tax rate is proposed to be ZAR120 per tonne of quantified CO_2 emissions and must be reported and paid on a half-yearly basis [25].

FeCr industries in SA are significant contributors to the total national GHG emissions [16, 26], and will therefore, according to the Carbon Tax Act (or "The Bill") [25], and the Department of Environmental Affairs [19], become liable for carbon tax. The ferroalloy production industry generates great volumes of off-gases, FeCr being the largest CO_2 producer of them all, as seen in Figure 1-2 [27].

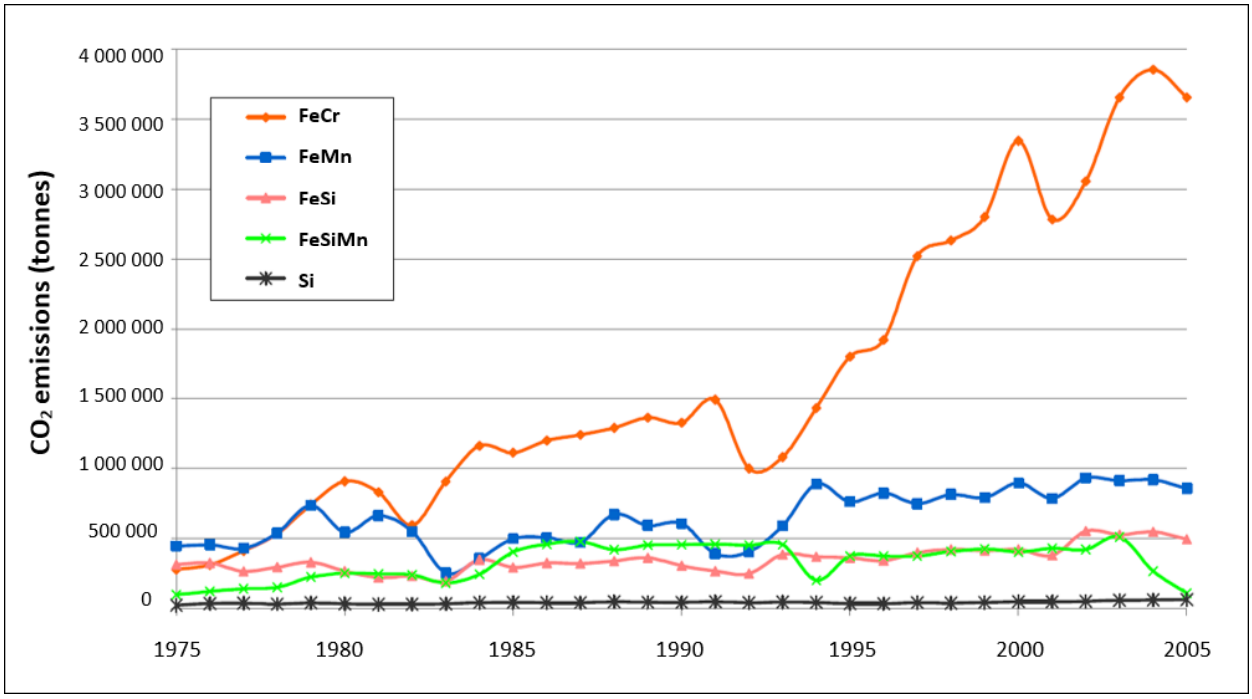


Figure 1-2: GHG emissions from ferroalloy production in SA

From Figure 1-2, it can be seen that the total CO_2 emissions estimation was approximately 3.6 Mt for 2005 [27]. Due to the increase of FeCr production (± 30% from 2005 to date [28, 29]), it can be assumed that the CO_2 emissions from FeCr production increased with a similar percentage. The estimated carbon tax risk is calculated to be R562 million per year (calculated in Equation 1-1 below), indicating that carbon tax will have a significant impact on SA FeCr industries due to the amount of emissions.

$$Carbon\ tax\ liability\ (R) = (3\ 600\ kt\ CO_2\ emissions + 30\%) \times \frac{R120}{t\ CO_2\ emissions} = R562\ million$$

Equation 1-1: Carbon tax liability

1.2. A new challenge

It seems likely that companies from the FeCr production industry will have to pay carbon tax in the near future[1]. According to recent studies, carbon tax is currently seen as a complex matter with several concerns and uncertainties regarding the implementation thereof [20, 22]. Industries affected (e.g. the FeCr industry) may have several questions regarding carbon tax. The first ones assumed to come to mind, are the following:

- *How should one quantify GHG emissions for FeCr production? (A)*
- *Are there practical examples available of FeCr emission calculations? (B)*
- *How can one be sure that the final result is correct? (C)*

In order to address these three initial questions (A – C), the official SA carbon tax documentation will be scrutinised for answers. The structure showed in Figure 1-3, developed by Gous [20], provides the regulatory landscape for carbon tax. The Bill [25] serves as the primary source of carbon tax, whereas the Benchmark Regulations [30], Offset Regulations [31], and GHG Reporting Regulations [32] serve as supporting documentation.

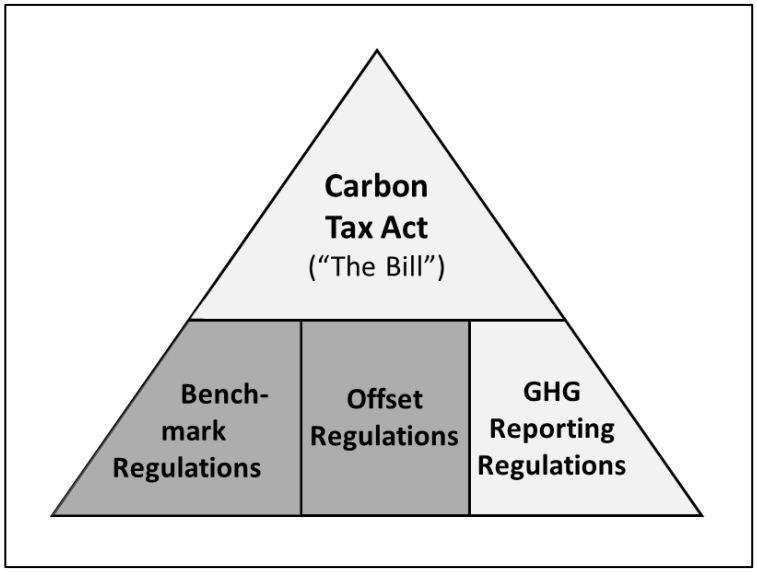


Figure 1-3: Basic regulatory landscape for carbon tax in SA

Due to the main focus being emissions and the quantification thereof, the two references, Benchmark Regulations and Offset Regulations, are not applicable. The Bill, as well as the GHG Reporting Regulations, will thus be analysed to evaluate whether any of the initial questions (*A* – *C*) are addressed.

[1] "Treasury must abandon carbon tax plan in light of IRP", *Engineering news*, 18 September 2018, Johannesburg.

The Bill

The first question (*A: How should one quantify GHG emissions?*) is not addressed with a high level of detail within The Bill [25]. The Bill simply states that a certain formula should be used in order to quantify the amount of GHG emitted in tonnes. This formula is given in Equation 1-2.

$$E = A \times B$$

Equation 1-2: GHG emission quantification methods (Draft Carbon Tax Bill)

Where,

"E" represents the number of GHG emissions to be determined, expressed in tonnes;

"A" represents the mass of any type of the fuel or product expressed in tonne; and

"B" represents the greenhouse gas emission factor in CO_2 equivalent tonnes per tonne of *A*.

The second question (*B: Are there practical examples available?*) is not addressed. No practical examples on how to quantify GHG emissions are provided in The Bill. The third question (*C: How can one be sure that the final result is correct?*) is also not addressed in The Bill.

The Bill mainly focuses on providing a holistic view on the general idea of carbon tax and the administration and legalities thereof, and doesn't necessarily focus on the calculation of the actual emissions. The document consists of six parts: I) *Definitions and general provisions relating to imposition of carbon tax*, II) *Allowances*, III) *Limitation of allowances*, IV) *Administration, tax period and payment of tax*, V) *Impermissible arrangements*, and VI) *Miscellaneous*, including the emission factors of various sources and processes [25]. Since The Bill does not address any of the identified uncertainties thoroughly, the next reference (GHG Reporting Regulations) will be analysed next in terms of questions A – C.

GHG Reporting Regulations

Question *A* is not directly addressed in the GHG Reporting Regulations [32]. No formulas or mathematical equations are provided where the estimation of GHG emissions are explained, as with The Bill. There is, however, reference to different "tiers". These tiers refer to different methods used to determine the GHG emissions. Even though definitions for each one of these tiers are given, no explanation / interpretation is provided.

The conclusion can be made that there are more than one method to calculate the GHG emissions from a specific process. This statement causes another question to arise, i.e., (*D) How do the methods ("tiers") differ from each other, and are there ways to improve prescribed methods?*

Question *B* is yet again not addressed. No practical examples on how to quantify GHG / CO_2 equivalent emissions are provided by the GHG Reporting Regulations. Question *C* is not fully addressed by the GHG Reporting Regulations, as there is no clear statement on how to evaluate accuracy of the results. No information or comparison is given by the GHG Reporting Regulations regarding the different tiers (question *D*).

After close evaluation of The Bill, together with the GHG Reporting Regulations, it was found that there are still several uncertainties concerning the initial questions/concerns (*A* – *D*). The Bill and the GHG Reporting Regulations, which form part of the national official carbon tax documentation, give a basic concept of carbon tax, but are overly generic, and do not give detailed information for FeCr specifically.

It is therefore necessary to do an in-depth critical literature study / additional literature in terms of the uncertainties identified (questions A – D). The hypothesis at this stage is that different emission quantification techniques will significantly affect the carbon tax liability of the FeCr industry. A critical literature evaluation is necessary in order to confirm this hypothesis.

1.3. Critical literature evaluation

A high-level layout of the regulatory carbon tax landscape was given in the previous section (Figure 1-3). Since the sources referred to within this landscape were not sufficient to address the uncertainties identified, it needs to be expanded to include non-official documents as well. Figure 1-4 shows the previous carbon tax documentation (from Figure 1-3), together with other significant documents referred to amongst carbon tax literature. The sources referred to in this landscape include the following (adapted from Gous [20]):

- *Carbon Tax Act* [25]
- *Benchmark Regulations* [30]
- *Carbon Offset Regulations* [31]
- *National GHG Reporting Regulations* [32]

Official carbon tax documentation (included in Figure 1-3)

- *Official Media Statement* [33]
- *Technical Guidelines for Monitoring, Reporting, Verification and Validation of GHG Emissions by Industry* [34]
- *IPCC Guidelines for National Greenhouse Gas Inventories (2006)* [35]

Each arrow represents one source referring to another, e.g. the Carbon Offset Regulations refer to the Carbon Tax Act, while the Carbon Tax Act refers to the IPCC Guidelines.

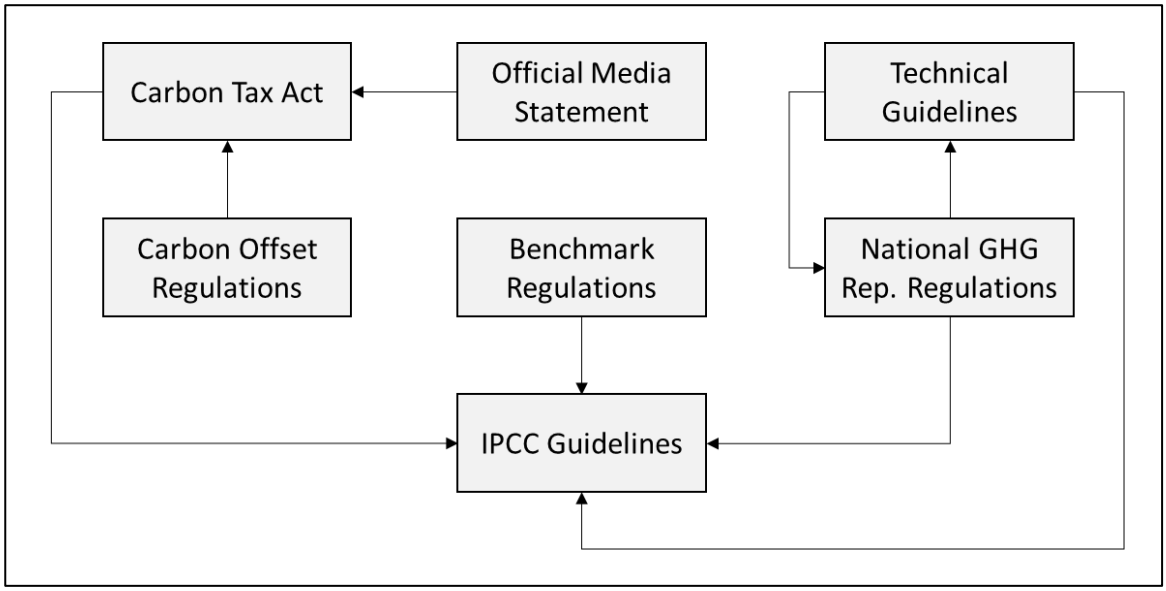


Figure 1-4: Relationship of documents associated with carbon tax and emission quantification

Except for the Media Statement, the remaining references provide guidance for interpreting and understanding GHG emissions occurring from industrial processes. The IPCC Guidelines for National Greenhouse Gas Inventories (hereafter referred to as IPCC Guidelines) are the rules established by the Intergovernmental Panel on Climate Change (IPCC) for the formation and conservation of national greenhouse gas inventories.

The Technical Guidelines for Monitoring, Reporting, Verification and Validation of Greenhouse Gas Emissions by Industry (hereafter referred to as Technical Guidelines) discuss the reporting methodology which is accepted by the competent authority on the website of National Department of Environmental Affairs. Since the associated carbon tax documentation from Section 1.2 was overly generic, these guidelines will be analysed next in terms of questions *A* – *D*, with the focus on FeCr emissions specifically.

IPCC Guidelines

The IPCC Guidelines provide information regarding industry-specific GHG emissions. Chapter 4.3 of these guidelines focuses exclusively on ferroalloy production, which includes ferrosilicon (FeSi), ferromanganese (FeMn), ferromolybdenum (FeMo), ferrovanadium (FeV), ferrotungsten (FeW), and of course, ferrochromium (FeCr) [35].

The IPCC Guidelines address Question *A* in more detail than with the previous two assessments. There are reference to the different “tiers”, or calculation methods, on how to quantify the GHG (specifically CO_2) emissions. Below are the equations given: tier 1 (Equation 1-3), tier 2 (Equation 1-4), and tier 3 (Equation 1-5) [35]:

Tier 1: Production-based emission factors

$$E_{CO_2} = \sum_i (MP_i \times EF_i)$$

Equation 1-3: Calculation method - Tier 1

Tier 2: Production-based, raw material specific emission factors

$$E_{CO_2} = \sum_i \left(M_{reducing\ agent,i} \times EF_{reducing\ agent,i}\right) + \sum_h (M_{ore,h} \times Ccontent_{ore,h}) \times \frac{44}{12} + \sum_j (M_{slag\ forming\ material,j} \times Ccontent_{slag\ forming\ material,j}) \times \frac{44}{12} - \sum_k \left(M_{product,k} \times Ccontent_{product,k}\right) \times \frac{44}{12} - \sum_l \left(M_{non-product\ outgoing\ stream,l} \times Ccontent_{non-product\ outgoing\ stream,l}\right) \times \frac{44}{12}$$

Equation 1-4: Calculation method - Tier 2

Tier 3: Calculations based on amounts and analyses of reducing agents

$$E_{CO_2} = \sum_i \left(M_{reducing\ agent,i} \times CContent_{reducing\ agent,i}\right) \times \frac{44}{12} + \sum_h (M_{ore,h} \times Ccontent_{ore,h}) \times \frac{44}{12} + \sum_j (M_{slag\ forming\ material,j} \times Ccontent_{slag\ forming\ material,j}) \times \frac{44}{12} - \sum_k \left(M_{product,k} \times Ccontent_{product,k}\right) \times \frac{44}{12} - \sum_l \left(M_{non-product\ outgoing\ stream,l} \times Ccontent_{non-product\ outgoing\ stream,l}\right) \times \frac{44}{12}$$

Equation 1-5: Calculation method - Tier 3

Where,

"E_{CO_2}" = CO_2 emissions from ferroalloy production, in tonnes

"*MPi*" = production of ferroalloy type *i*, in tonnes

"*EFi*" = generic emission factor for ferroalloy type *i*, in tonnes CO_2 / tonne ferroalloy product

"$M_{reducing\ agent,\ i}$" = mass of reducing agent *i*, in tonnes

"$EF_{reducing\ agent,\ i}$" = emission factor of reducing agent *i*, in tonnes CO_2 / tonne reducing agent

"$CContent_{reducing\ agent,\ i}$" = carbon (C) content in reducing agent *i*, in tonnes C/tonne reducing agent

"$M_{ore,\ h}$" = mass of ore *h*, in tonnes

"$CContent_{ore,\ h}$" = C content in ore *h*, in tonnes C/tonne ore

"$M_{slag\text{-}forming\ material,\ j}$" = mass of slag-forming material *j*, in tonnes

"$CContent_{slag\text{-}forming\ material,\ j}$" = C content in slag-forming material *j*, in tonnes C/tonne material

"$M_{product,\ k}$" = mass of product *k*, in tonnes

"$CContent_{product,\ k}$" = C content in product *k*, in tonnes C/tonne product

"$M_{non\text{-}product\ outgoing\ stream,\ l}$" = mass of non-product outgoing stream *l*, in tonnes

"$CContent_{non\text{-}product\ outgoing\ stream,\ l}$" = C content in non-product outgoing stream *l*, in tonnes C/tonne

The constant factor $\frac{44}{12}$ represents the number which should be multiplied with the amount of total carbon used in order to calculate the mass of CO_2 emitted [35] (molecular weight of C = 12 g/mol, O = 16 g/mol, CO_2 = 44 g/mol [36]).

A visual representation developed by Booysen [22] illustrates certain details of each tier in a pyramid structure. This is shown in Figure 1-5.

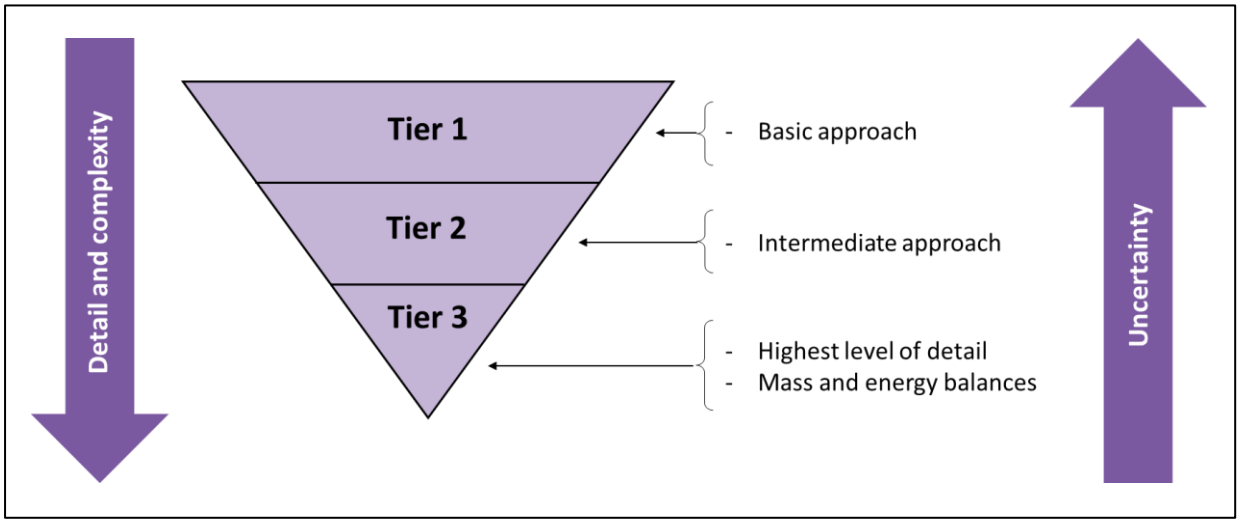


Figure 1-5: Comparative structure of prescribed tiers (developed by Booysen)

The figure clearly indicates that, as the details and complexity increase, the uncertainty of the methods decreases. Tier 1 (top of the pyramid structure) is the most basic approach, and uses an internationally-based emission factor to determine the emissions. Tier 2 requires more detail than tier 1, and makes use of national or country-specific emission factors. Tier 3 (bottom of the pyramid) is the most complex method. It uses a mass-balance approach together with facility specific carbon contents, if available [22, 35].

Even though these mathematical equations are given, no detailed explanation or interpretation is provided. These are also generic for all ferroalloys, and not exclusive to ferrochrome specifically. No practical or real-life examples for quantifying the emissions are provided within the IPCC Guidelines. Thus, question *B* is yet again not addressed.

Question *C*, which deals with uncertainty *(How can one be sure that the final result is correct?)*, is addressed briefly by the IPCC Guidelines. Any uncertainties regarding the production of ferroalloys would result from either the uncertainty related to the activity data, or from the emission factor. The following tables summarise the quantified uncertainty associated with the two parameters, activity data, and emission factors (Table 1-2 and Table 1-3, respectively) [35]:

Table 1-2: Uncertainty ranges for activity data used in ferroalloy emission quantifications

Method	Data source	Uncertainty
Tier 1	National production data	< 5%
	Default emission factors	< 25%
Tier 2	Company-derived reducing agent and process materials	< 5%
	National reducing agent and process materials data	< 5%
	Company-specific emission factors	< 5%
	Material-specific default emission factors	< 10%
Tier 3	Company-specific measured CO_2 data	< 5%

Table 1-3: Uncertainty ranges for emission factors used in emission quantifications

Method	Uncertainty
Tier 1	25% - 50%
Tier 2	±10%
Tier 3	< 5%

These uncertainty values and ranges indicate to which extent one can be sure of the final answer. However, it does not directly/clearly state how one can be assured that the final result is correct, or how one can manage the uncertainties.

Question *D* addresses the issue: *How do the methods ("tiers") differ from each other and are there ways to improve prescribed methods*? The only comparison available between the different tiers is under the section of uncertainty assessment in the IPCC Guidelines (referred to this section in Table 1-2 and Table 1-3). There are, therefore, no other comparisons or ways of improving these methods stated in the IPCC Guidelines.

*[Footnote: A possible 50% error on R562 million (risk in Section 1.1) = total risk of **R843 million**]*

Technical Guidelines

According to Figure 1-4, the Technical Guidelines often refer to the IPCC Guidelines for information on GHG emissions from the ferroalloy production industry. The Technical Guidelines therefore do not provide any significant additional information to that of the IPCC Guidelines [34, 35].

Since the IPCC Guidelines and the Technical Guidelines do not address all of the questions thoroughly, the documents referred to in the IPCC Guidelines (Fe-alloy section, 4.3) will be analysed lastly in terms of questions *A – D.* These references include the following:

- *CO_2 emissions from the production of Mn and Cr alloys (Olsen et al., 1998)* [37]
- *Greenhouse gas emissions from ferroalloy production (Lindstad et al., 2006)* [38]

Olsen et al.; Lindstad et al.

Since the IPCC guidelines are written by using these references, the four questions (*A – D*) are not addressed in any more detail by Olsen *et al.* [37] or Lindstad *et al.* [38] than in the IPCC Guidelines [35].

There are, however, reference to different types of furnaces. Closed, semi-closed and open furnaces are discussed, as well as alternating current (AC) and direct current (DC) arc furnaces. This statement causes another question to arise, i.e., *(E) How would the different furnace technologies influence the emissions?*

After having evaluated all references previously discussed, it appears that tier 3 would require significantly more effort, and be more time consuming and intricate than tier 1 or 2. This causes the final question to arise, i.e., *(F) Will it be worthwhile to go through that level of detail and effort to get to a quantified number of emissions?*

The figure below (Figure 1-6) summarises the references scrutinised in Section 1.2 and 1.3 for clarity around the emissions quantification from the FeCr industry [25, 32, 34, 35, 37, 38].

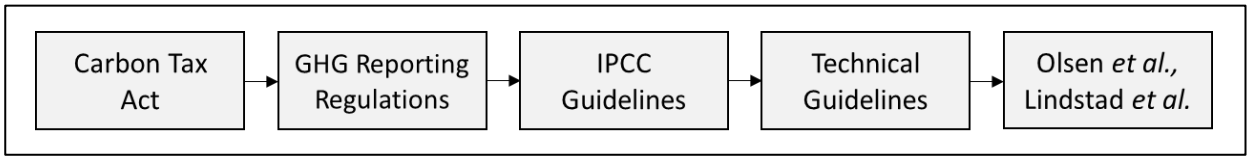


Figure 1-6: References scrutinised for clarity around GHG emissions from FeCr production

From the start of Section 1.2, there were three initial questions regarding the quantification of GHG emissions from the FeCr production process. Official/legal documentation was scrutinised to address these questions. However, this lead to even more uncertainty, as the uncertainties increased from three to six questions. To summarise, these questions include the following:

(A) How should one quantify GHG emissions for FeCr production?
(B) Are there practical examples available of FeCr emission calculations?
(C) How can one be sure that the final result is correct?
(D) How do the methods ("tiers") differ from each other, and are there ways to improve prescribed methods?
(E) How would the different furnace technologies influence the emissions?
(F) Will it be worthwhile to go through that level of detail and trouble to get to a quantified number of emissions?

Since these uncertainties could not be resolved or thoroughly addressed by any of the references used, a full reference trail will be developed to be scrutinised yet again in order to gain clarity on the six uncertainties identified. This reference trail was developed by using two independent starting points (carbon tax, and the ferroalloy industry), and collecting over a 100 relevant references. Figure 1-7 shows this reference trail.

The references from Figure 1-7 will be used to complete the critical review for the uncertainties associated with the emission quantification of FeCr production. This critical review will take place in two phases: *Critical review – Phase 1*, and *Critical review – Phase 2*.

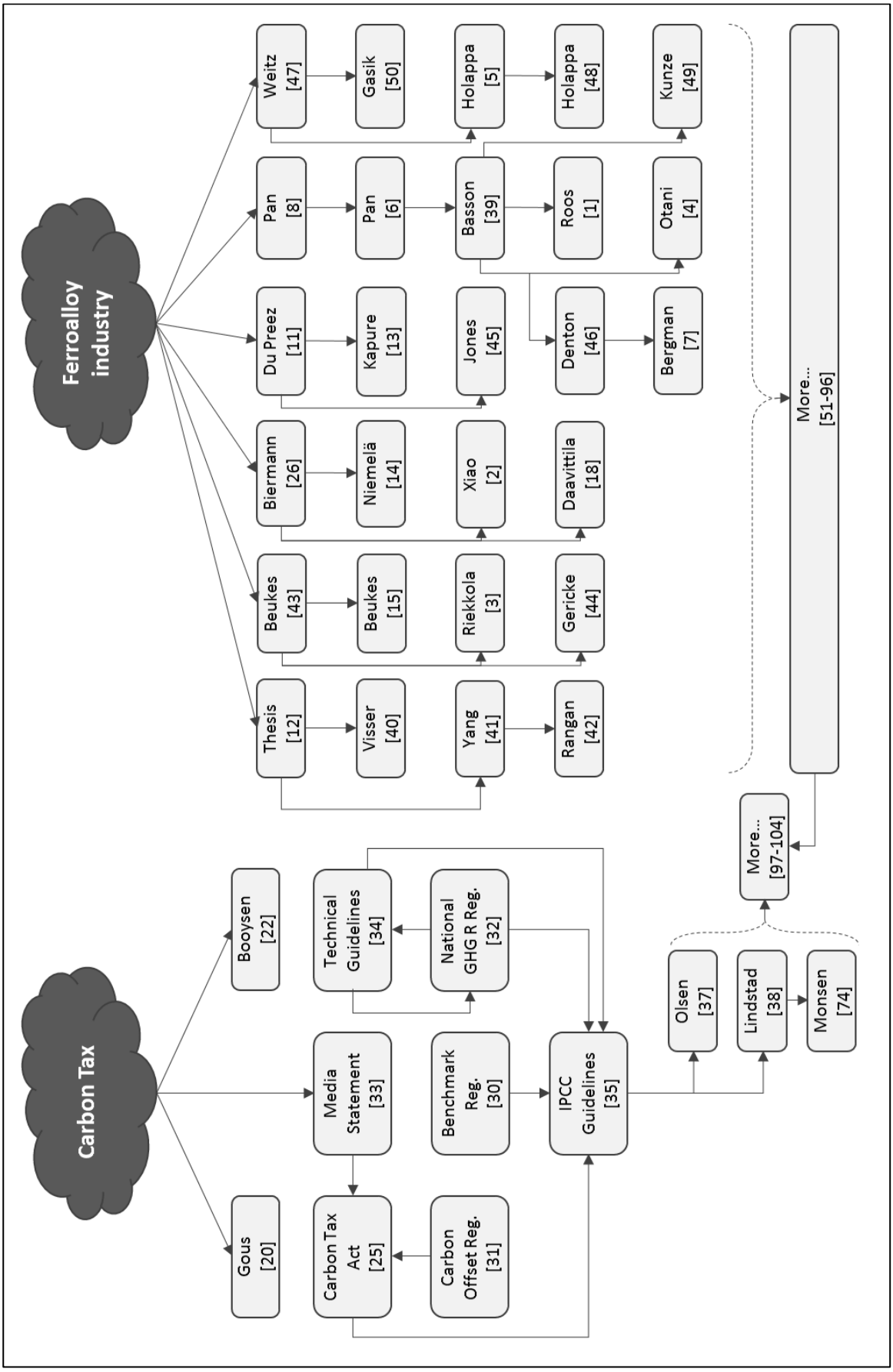


Figure 1-7: Reference trail including carbon tax and the ferroalloy industry

Critical review - Phase 1

The 104 references identified in the reference trail from Figure 1-7 are evaluated thoroughly to gain a basic knowledge and understanding of carbon tax, the ferroalloy industry and GHG emissions from ferroalloy (and specifically, FeCr) production. These references are of decent quality, consisting mostly of academic dissertations or theses, journal articles, conference papers, and official or legal documentation. The distribution of reference types can be seen in Figure 1-8.

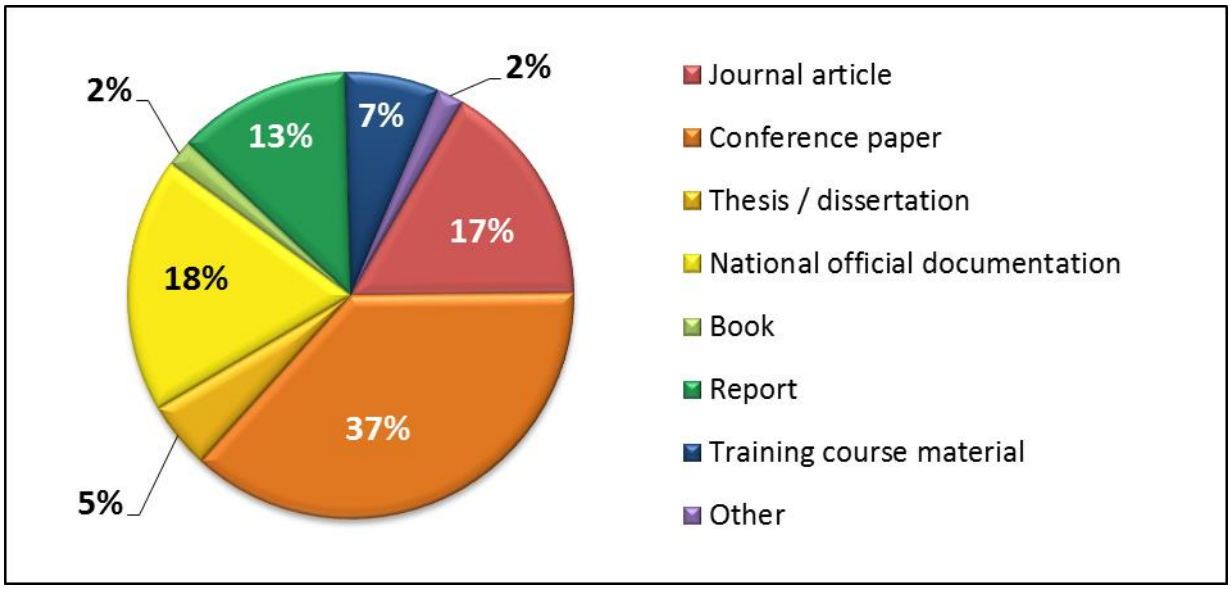


Figure 1-8: Reference type distribution (Phase 1)

Next, the references will be categorised according to their focus of study, i.e. energy, production, economics, modelling, environment and emission quantification. The categorisation of references of Phase 1 can be seen in Appendix A (Table A-2). The 104 references were scrutinised in terms of their relevance to ferrochrome emissions, or emission quantification in general. Thereafter, only the relevant sources are selected to proceed to Phase 2 for assessment.

Critical review - Phase 2

From the 104 references assessed (Phase 1), only 36 were selected for further evaluation, based on the final questions. Again, the majority of these 36 references can be considered reliable sources, including journal articles, conference papers, theses or dissertations, national official documentation and published reports (Figure 1-9).

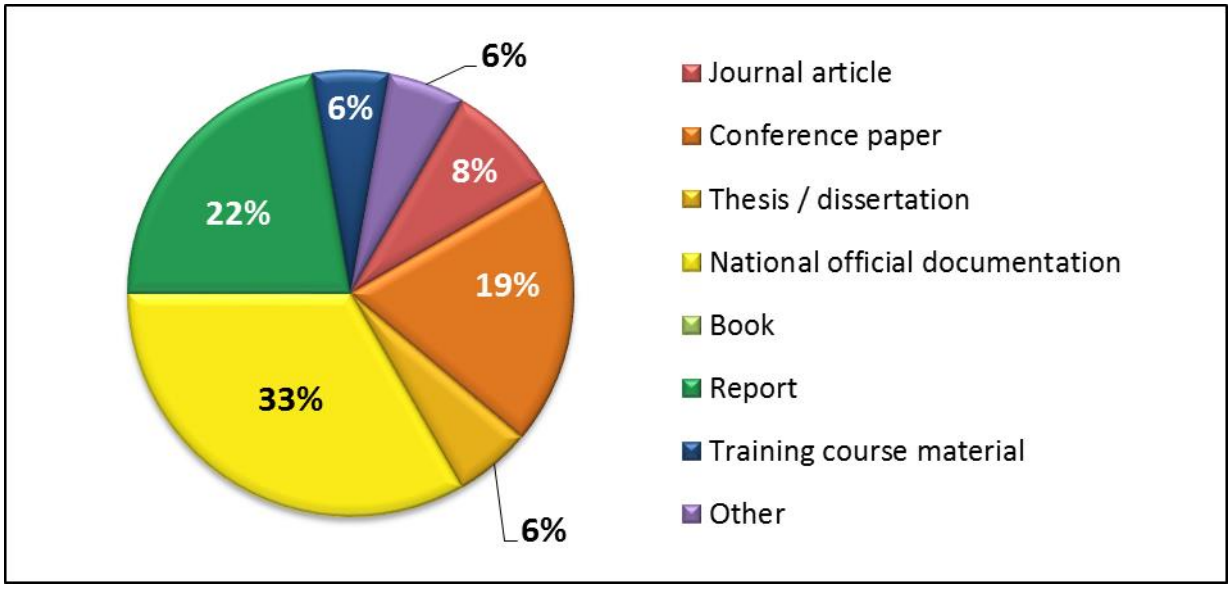


Figure 1-9: Reference type distribution (Phase 2)

These 36 selected references will be examined based on the six final questions listed on page 12:

(A) How should one quantify GHG emissions for FeCr production?

(B) Are there practical examples available of FeCr emission calculations?

(C) How can one be sure that the final result is correct?

(D) How do the methods ("tiers") differ from each other, and are there ways to improve prescribed methods?

(E) How would the different furnace technologies influence the emissions?

(F) Will it be worthwhile to go through that level of detail and trouble to get to a quantified number of emissions?

Table 1-4 indicates the symbol "X" when the specific reference addresses the uncertainty (*A* – *F*).

Table 1-4: Phase 2 of critical literature review

Reference	Type of ref.	Does reference address the following uncertainty?						Ref. nr. *(ref. list)*
		(A)	***(B)***	***(C)***	***(D)***	***(E)***	***(F)***	
ADEME	N/OD							[93]
APTA	N/OD							[94]
Booysen	JA	X						[22]
CAPCOA	N/OD							[95]
Chen & Johnson	R							[96]
Chesnokov	JA							[52]
Defra	R							[97]
Dept. of environmental affairs	N/OD	X		X				[19]
Dept. of environmental affairs	R	X						[32]
Environmental protection act	R	X						[107]
EPA	N/OD	X						[54]
Gous	T/D			X				[20]
Holappa	CP	X						[5]
IPCC	N/OD			X				[35]
IPCC	R	X						[99]
IPIECA	R							[100]
Koekemoer	CP	X						[67]
Lindstad	CP	X						[16]
Lindstad	CP	X						[38]
Merafe	N/OD	X						[71]
Metallurgical industry	Other	X						[72]
Milne et al.	JA	X						[102]
Monsen	CP	X						[74]
NAPCA	N/OD							[76]
Niemelä	CP	X						[14]
NPI	N/OD	X						[78]
Olsen	CP	X						[37]
PMR	TCM			X				[110]
Sonntag-O'Brien	TCM							[103]
The Norwegian Emission Inv.	N/OD	X						[109]
UNFCCC Reporting Guidel.	N/OD	X						[17]
US EPA	N/OD	X						[86]
Vaish	Other	X						[87]
Vellinga	R							[108]
Weitz	T/D	X						[47]
Young	R							[104]

**T/D – thesis/dissertation, JA – journal article, CP – conference paper, N/OD – national or official documentation, TCM – training course material, R - report, B - book.*

It is clear to see that neither questions *B, D, E,* nor *F* are thoroughly addressed in any of the works evaluated. It is thus safe to assume that information regarding these uncertainties are not widely available in literature, and therefore certain gaps within FeCr emission quantification literature can be recognised. Table 1-5 is a duplication of Table 1-4, with additional indication of how the main focus areas of this study were identified. These are indicated by the yellow blocks stating "Focus area 1", "Focus area 2", or "Focus area 3".

Table 1-5: Identifying the focus areas of the study based on Phase 2

Reference	Type of ref.	Does reference address the following uncertainty?						Ref. nr. *(ref. list)*
		(A)	*(B)*	*(C)*	*(D)*	*(E)*	*(F)*	
ADEME	N/OD		Focus area 1		Focus area 2	Focus area 3		[93]
APTA	N/OD							[94]
Booysen	JA	x						[22]
CAPCOA	N/OD							[95]
Chen & Johnson	R							[96]
Chesnokov	JA							[52]
Defra	R							[97]
Dept. of environmental affairs	N/OD	x		x				[19]
Dept. of environmental affairs	R	x						[32]
Environmental protection act	R	x						[107]
EPA	N/OD	x						[54]
Gous	T/D			x				[20]
Holappa	CP	x						[5]
IPCC	N/OD			x				[35]
IPCC	R	x						[99]
IPIECA	R							[100]
Koekemoer	CP	x						[67]
Lindstad	CP	x						[16]
Lindstad	CP	x						[38]
Merafe	N/OD	x						[71]
Metallurgical industry	Other	x						[72]
Milne et al.	JA	x						[102]
Monsen	CP	x						[74]
NAPCA	N/OD							[76]
Niemelä	CP	x						[14]
NPI	N/OD	x						[78]
Olsen	CP	x						[37]
PMR	TCM			x				[110]
Sonntag-O'Brien	TCM							[103]
The Norwegian Emission Inv.	N/OD	x						[109]
UNFCCC Reporting Guidel.	N/OD	x						[17]
US EPA	N/OD	x						[86]
Vaish	Other	x						[87]
Vellinga	R							[108]
Weitz	T/D	x						[47]
Young	R							[104]

From Table 1-5, three different focus areas were identified based on the lack of literature regarding questions/uncertainties *B, D, E* and *F*. Each of these focus areas will be developed into an individual chapter in this thesis, with the aim to address the uncertainties identified.

Uncertainty not addressed by literature from Table 1-5: *Are there practical examples available of FeCr emission calculations?* Focus area 1 was identified due to the lack of practical examples available in literature. A practical application of the existing, or prescribed, methods will be implemented on actual FeCr industries, in order to address the uncertainty identified (*B*).

Uncertainty not addressed by literature from Table 1-5: *How do the methods ("tiers") differ from each other, which one is the best, and are there any other options, or ways to improve prescribed methods?* Focus area 2 was identified to evaluate the possibility of improving the current calculation methods, or tiers. Since tier 3 is the most detailed method, it will be refined to investigate any possible further improvements on the prescribed methods (*D).*

Uncertainty not addressed by literature from Table 1-5: *How would the different furnace technologies influence the emissions?* W*ill it be worthwhile to go through a high level of detail and trouble (tier 3) to get to a quantified number of emissions?* Since no information could be found regarding how the different types of FeCr furnaces would affect the amount of CO_2 emitted, the third and final focus area was identified. Also, having to use a method requiring more time and effort, but not giving a more accurate answer, is another fundamental concern. Thus, the different methods (prescribed and newly developed) will be compared throughout this focus area.

1.4. Problem statement

FeCr furnaces are responsible for a significant amount of GHG emissions. The proposed carbon tax for South Africa (implementation set for 2019) presents an estimated potential risk of R562 million (however, R843 million when considering the potential 50% uncertainty) per year for the local FeCr industry. This is a significant risk which will require detailed assessment.

Unfortunately the literature evaluation showed that there are no detailed analyses available on how the practical and operational reality will affect the results produced by the prescribed methods. It is therefore necessary to perform a critical analysis of the emission quantification methods to determine the associated risks for the ferrochrome industry. This main problem can be broken down into three smaller problems, and will be addressed throughout the document in three specific chapters (focus areas):

Focus area 1:

The core problem is that, since carbon tax has not been implemented, it is not yet fully understood and no practical examples on how to apply different methods are available. The need is thus to illustrate the practical application of the different prescribed calculation methods. This will be addressed in chapter 2: “PRACTICAL APPLICATION OF PRESCRIBED METHODS”.

Focus area 2:

There are currently three calculation methods of quantifying CO_2 emissions from FeCr production. As stated in Section 1.3, these methods are not necessarily accurate. However, there is no system in place to practically improve on these prescribed methods. There is a need to refine these prescribed methods and investigate the potential for improvement. This will be addressed in chapter 3: “REFINEMENT OF PRESCRIBED METHODS”.

Focus area 3:

The accuracy and practicality of different approaches are unknown. Based on the knowledge gained from the critical literature review, the complexity of tier 1, 2, and 3 would differ significantly. There is a concern, however, that even though some of these methods are more complex, they do not necessarily provide “better”, or more accurate, results. There is thus a need to investigate and compare the complexity and accuracy of the different methods (prescribed and developed). This will be addressed in Chapter 4: “COMPARISON OF DIFFERENT METHODS”.

1.5. Contributions of study

This thesis undertakes to provide several novel contributions to the field of emission quantification in the FeCr industry. These contributions are grouped into three categories: critical assessments, development of practical methods, and the quantification of implications for the SA FeCr industry.

Critical assessments of literature and operational information to establish links, identify risks, and devise solutions. The thesis produces novel contributions by assessing:

- The legal landscape and national and international resources available to the FeCr industry to highlight the lack of practical applications and examples.
- Literature to establish a link between the prescribed legal processes and what is available from real-world operational systems.
- The prescribed methods to highlight several practical constraints associated.
- Available furnace characteristics from the iron- and steel industry for an application to quantify FeCr slag mass.
- Coal composition analyses to determine the feasibility of practically determining the carbon content of the reductant, based on operational measurements.

(Discussed in Section 5.2.1)

The presented research and subsequent critical assessments produced several risk areas and linked these to feasible solutions. This thesis produces novel contributions by incorporating its research findings into several practical methods to:

- Apply prescribed methods to real-world furnaces.
- Link compositional analyses to mass measurements.
- Perform mass balances in order to systematically go from general to specific data with the aim to improve accuracy.
- Quantify and compare the accuracy and complexity associated with FeCr carbon tax calculations.

(Discussed in Section 5.2.2)

The presented research, critical assessments and subsequent practical methods are highly valuable and applicable to the wider FeCr industry. This thesis further contributes specifically to the South African FeCr industry by producing tangible results which brings significant insight and value to the field of study. This document specifically quantifies:

- The impact of operational errors

- The accuracy change in mass balances
- The variances between the different methods
- The complexities of the different methods
- The estimated industry exposure (SA FeCr carbon tax liability)

(Discussed in Section 5.2.3)

The novelty of this thesis lies in the approach of using critical analyses to identify risks and possible solutions. These risks and solutions are then reconciled by developing practical methods that are both applicable and usable to industry. Finally, the impact of the work is quantified by using multiple case studies. The results verify the functionality of the approach, but also validates the value and significance for South Africa's FeCr industry.

More detail on how each contribution was accomplished is available in Chapter 5 (Section 5.2).

1.6. Outline of document

Chapter 1 gives relevant background information on FeCr furnaces and the associated emissions. Some uncertainties are identified in the form of research questions, which leads to an in-depth critical literature review, whereafter certain gaps are identified. The gaps become the three focus areas of the study, and are discussed and addressed in Chapters 2, 3 and 4.

Chapter 2 highlights the problem of how the application of carbon tax calculations is not yet fully understood and how no sufficient practical examples of the application of different methods are available. Case studies are used to practically apply these prescribed calculation methods and illustrate the significance of every step in the methodology developed. It also gives an indication of the risk associated with some practical constraints.

Chapter 3 explores the opportunity to refine the prescribed methods from literature and investigate the potential for improvement. The prescribed methods are refined by making use of advanced mass balance techniques.

Chapter 4 reviews the results from Chapter 2 and Chapter 3 and investigates and compares the variance, accuracy and complexity of the different quantification methods (prescribed and developed). This is done by applying the different methods to 17 South African FeCr producing furnaces. The results from all case studies are validated in this chapter.

Chapter 5 concludes the study, discusses the novelty contributions and provides recommendations for future work.

2. PRACTICAL APPLICATION OF PRESCRIBED METHODS

2.1 Introduction

Carbon tax has not yet been implemented and is not fully understood. The critical study from Chapter 1 showed that no detailed practical examples on how to apply the different prescribed quantification methods, or "tiers" (hereafter referred to as the "prescribed methods"), are found in literature. Hence, there is a need to illustrate the practical application of these prescribed methods.

This chapter will illustrate the calculation of the emissions from FeCr production based on the prescribed methods. In addition to this, the chapter will also highlight several potential constraints that may occur during the practical application of these methods, which will also be the focus of the case studies provided. These case studies will quantify the potential impact of these constraints on the final carbon tax results. It is expected that the potential constraints will have a significant effect on the final CO_2 results.

2.2 Literature study

2.2.1 Preamble

The literature study will present a solid framework from which the methodology in Section 2.3 will be developed. The prescribed methods will be rehashed to understand what is required for the relevant calculations (Section 2.2.2). A brief discussion of the FeCr process and its typical measurements will highlight the primary overview of the FeCr industry key performance indicators (KPIs) in Section 2.2.3 and 2.2.4. Lastly, data quality evaluation techniques will be reviewed to improve on the quality of any dataset received from site (Section 2.2.5). This section will be concluded in Section 2.2.6.

2.2.2 Prescribed quantification methods

According to the research conducted in Chapter 1, there are three prescribed methods on how to quantify the GHG (specifically CO_2) emissions from FeCr production, called "tiers":

- *Tier 1: Production-based emission factors*
- *Tier 2: Production-based, raw-material-specific emission factors*
- *Tier 3: Calculations based on amounts and analyses of reducing agents*

These methods are presented in Equation 1-3, Equation 1-4 , and Equation 1-5, in Section 1.3, and are repeated on the next page.

Tier 1: *(repeat of Equation 1-3)*

$$E_{CO_2} = \sum_i (MP_i \times EF_i)$$

Tier 2: *(repeat of Equation 1-4)*

$$E_{CO_2} = \sum_i \left(M_{reducing\ agent,i} \times EF_{reducing\ agent,i}\right) + \sum_h (M_{ore,h} \times Ccontent_{ore,h}) \times \frac{44}{12} + \sum_j (M_{slag-forming\ material,j} \times Ccontent_{slag-forming\ material,j}) \times \frac{44}{12} - \sum_k \left(M_{product,k} \times Ccontent_{product,k}\right) \times \frac{44}{12} - \sum_l \left(M_{non-product\ outgoing\ stream,l} \times Ccontent_{non-product\ outgoing\ stream,l}\right) \times \frac{44}{12}$$

Tier 3: *(repeat of Equation 1-5)*

$$E_{CO_2} = \sum_i \left(M_{reducing\ agent,i} \times CContent_{reducing\ agent,i}\right) \times \frac{44}{12} + \sum_h (M_{ore,h} \times Ccontent_{ore,h}) \times \frac{44}{12} + \sum_j (M_{slag-forming\ material,j} \times Ccontent_{slag-forming\ material,j}) \times \frac{44}{12} - \sum_k \left(M_{product,k} \times Ccontent_{product,k}\right) \times \frac{44}{12} - \sum_l \left(M_{non-product\ outgoing\ stream,l} \times Ccontent_{non-product\ outgoing\ stream,l}\right) \times \frac{44}{12}$$

The variables referred to by these equations for quantifying the CO_2 emissions include:

- the **mass** of the **input streams** [ore ($M_{ore,\ h}$), reducing agent ($M_{reducing\ agent,\ i}$), and slag-forming material, or "fluxes" ($M_{slag\text{-}forming\ material,\ j}$), in tonnes],
- the **mass** of the **product streams** [FeCr metal ($M_{product,\ k}$) and non-product outgoing stream, or "slag" ($M_{non\text{-}product\ outgoing\ stream,\ l}$), in tonnes],
- the **carbon content** of all streams [reducing agent ($CContent_{reducing\ agent,\ i}$), ore ($CContent_{ore,\ h}$), fluxes ($CContent_{slag\text{-}forming\ material,\ j}$), and FeCr metal ($M_{product,\ k}$), as a fraction], and
- universal emission factors (EFi, $EF_{reducing\ agent,\ i}$).

The two universal/generic emission factors (EFs) are not measured on site, and should be acquired from literature. The first EF (EFi) is fixed for all FeCr industries, as provided by the IPCC [35].

The EF would differ depending on the presence of a pelletising and sintering plant (PSP). As for the reducing agent EF ($EF_{reducing\ agent,\ i}$), the IPCC Guidelines suggest that inventory compilers use producer-specific values, which are based on the average blend of coal and/or coke for the specific site. However, this is rarely available, thus these values were found in literature from various sources. Table 2-1 and Table 2-2 give these values for EF_i and $EF_{reducing\ agent}$, respectively.

Table 2-1: Generic emission factor for ferrochrome production

Symbol	Unit	Without PSP	With PSP
EFi	Tonnes CO_2 / tonne ferroalloy product	1.3	1.6

Table 2-2: Generic emission factor for reducing agents

Symbol	Unit	Reference A [118]	Reference B [119]
$EF_{reducing\ agent,\ i}$	Tonnes CO_2 / tonne reducing agent		
Coal		2.96	2.325
Coke		3.21	2.819
Anthracite		-	2.602

Table 2-3 provides a summary of all data required by each of the prescribed methods.

Table 2-3: Data required for prescribed quantification methods

Data required for CO_2 quantification methods *(Information gathered from Section 1.3 and 2.2.2)*		
Tier	**Symbol used in tier equations**	**Description**
Tier 1	*MPi*	Production of ferroalloy *i*
	EFi	Generic emission factor for ferroalloy *i*
Tier 2	$EF_{reducing\ agent,\ i}$	Emission factor of reducing agent *i*
Tier 3	$CContent_{reducing\ agent,\ i}$	Carbon content in reducing agent *i*
Tier 2 and Tier 3	$M_{reducing\ agent,\ i}$	Mass of reducing agent *i*
	$M_{ore,\ h}$	Mass of ore *h*
	$CContent_{ore,\ h}$	Carbon content in ore *h*
	$M_{slag\text{-}forming\ material,\ j}$	Mass of slag-forming material *j*
	$CContent_{slag\text{-}forming\ material,\ j}$	Carbon content in flux *j*
	$M_{product,\ k}$	Mass of product *k*
	$CContent_{product,\ k}$	Carbon content in product *k*
	$M_{non\text{-}product\ outgoing\ stream,\ l}$	Mass of slag *l*
	$CContent_{non\text{-}product\ outgoing\ stream,\ l}$	Carbon content in slag *l*

It seems fairly straightforward to apply these prescribed methods based on the equations and the descriptions above. This is, in fact, the case if you know what data to use, and if the required data

is available and correct. If the data is not available for a certain prescribed method, this calculation can simply not be completed. There are also possible risks when applying the prescribed methods. In order to use these prescribed methods to estimate the CO_2 emissions as accurately as possible, it is important to understand the FeCr production process, the significant measurement points, as well as obtaining and using the relevant data (Sections 2.2.3, 2.2.4, and 2.2.5).

2.2.3 Ferrochrome process

As previously stated in Chapter 1, the production of ferrochrome is accomplished by feeding raw materials (chromite ores, reductant and fluxes) to an arc furnace [10, 11, 39]. In some cases, the raw materials are prepared before being fed to the furnace: pelletising, sintering and drying techniques are often performed on raw materials to produce a dry and uniform feed to the furnace, which would increase furnace stability [26, 120]. Pelletising and sintering of the raw materials are achieved at the pelletising and sintering plant (PSP).

Electricity is used to heat up the furnace and melt the raw materials by means of an electric arc [5, 12]. Due to the heat provided, various chemical reactions take place, causing reduction of the metal oxides within the chromite ore to a final metal product, FeCr. Together with the metal product (FeCr), slag and off-gas also exit the furnace as by-products [13]. Figure 2-1 illustrates this process [3].

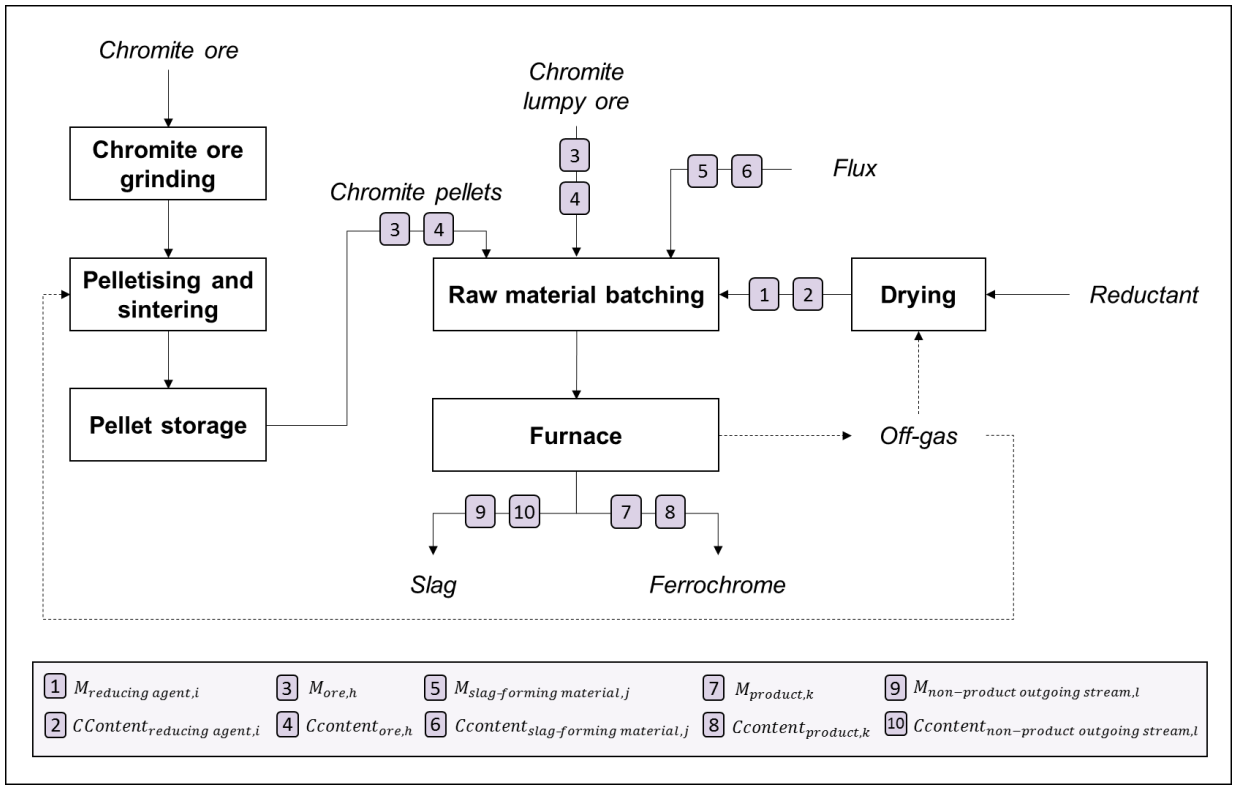


Figure 2-1: Ferrochrome production process

In Figure 2-1, some streams are labelled with purple tags, numbered from 1 to 10. The legend at the bottom of this figure gives a description of each tag, referring back to the variables required by the prescribed methods (as given by Equation 1-3, Equation 1-4 and Equation 1-5, and summarised in Table 2-3). This diagram has been summarised to shift the focus to the FeCr furnace, input, and output streams specifically. A simplified illustration of this process can be found in Figure 1-1 (Chapter 1).

2.2.4 Typical measurements

According to the prescribed methods, the data of specific parameters are required for calculations. Not all parameters are deemed crucial in the ferrochrome industry, and are therefore not always measured at the furnaces [121]. It is, however, important that certain streams are known. The measurements typically available for the general furnace will be discussed briefly:

FeCr metal product

The main objective of the process referred to in this study is the production of FeCr metal with a certain alloy grade. The mass and composition of the metal produced is therefore usually monitored closely and measured continuously [121]. The metal is tapped a few times per day, solidified, crushed, and then weighed on weighbridges[2]. Metal samples are also sent for regular (usually daily) composition analysis. A typical composition of the FeCr product is as follows: 56.7% Cr, 33.8% Fe, 7.2% C, and 2.3% Si [7].

Raw materials

The mass of raw materials (chromite ore, reductant and fluxes) are usually measured at weigh bins before being batched to the furnace [122]. The composition, however, is rarely known on site. Occasional sampling of the reductants takes place on site. However, this is generally done long before batching (before materials are stored on stockpiles), creating a significant buffer capacity. From literature, the composition of each of the raw materials normally used in FeCr production is summarised below:

Cr ore: 50% Cr_2O_3, 25% FeO, 9% MgO, 10% Al_2O_3, 5% SiO_2, 1% CaO [7]
Anthracite: 88.94% C, 3.4% H, 2.32% O, 1.55% N, 0.8% S [123]
Char: 77.8% C, 0.34% H, 21.11% O, 0.71% N [124]
Coke: 89% C, 3.6% H, 1.56% H, 4.95% S [125]
Coal: 76.7% C, 4.69% H, 10.5% O, 1.4% N, 0.4% S [123]
Dolomite: 100% $CaMg(CO_3)_2$ [126]

[2] Knowledge gained from site experience and interviews with site personnel

Limestone: 100% $CaCO_3$ [127]
Quartz: 100% SiO_2 [128]
Burnt lime: 100% CaO [129]

By-products

The two by-products (slag and off-gas) are often considered waste streams, and are rarely measured accurately[3]. The slag composition is, however, estimated to ensure the required slag composition [64]. From time to time, the slag mass is calculated by using a slag-to-metal ratio (usually between 1.1 and 1.8 tonne of slag produced per tonnes of metal [130]), which is estimated by random sampling. The amount of slag produced can also be estimated based on an aluminium (Al_2O_3) balance. This is done with the assumption that the slag analysis is done accurately and representatively [77]. The slag and off-gas compositions are given below:

Slag: 23.2% SiO_2, 24.7% Al_2O_3, 19.8% MgO, 3.0% CaO, 10.7% FeO, 18.6% Cr_2O_3 [77]
Off-gas: 75-90% CO, 2-10% CO_2, 2-15% H_2, 2-7% N_2 [15, 14]

Carbon contents of materials

The typical compositions of inlet and outlet streams are converted to element-based compositions by using the molecular weight of each formula and element (see Appendix C: Equation B-1 and Equation B-2). The results of the carbon content of each material (which are required for the calculation of CO_2 emission prescribed quantification methods) are summarised in Table 2-4:

Table 2-4: Typical compositions for all streams of a FeCr furnace (element-based)

Material *Raw (input), or product (output)*	**Carbon content (%)**	**Unit**
Chrome ore	-	
Anthracite	88.9	Mass %
Char	77.8	Mass %
Coke	89.0	Mass %
Coal	76.7	Mass %
Dolomite	13.0	Mass %
Limestone	12.0	Mass %
Quartz	-	
FeCr metal	7.2	Mass %
Slag	-	
Off-gas	33 - 41	Volume %

[3] Knowledge gained from site experience and interviews with site personnel

Table 2-5 (repeat of Table 2-3), provides a summary of all data required by the prescribed methods. An additional column has been added, stating whether or not these parameters are usually known on site. The reason why a parameter would not be measured on site is typically because of financial reasons, or the fact that it is not deemed an important parameter.

Table 2-5: Data required for prescribed quantification methods

Data required for CO_2 quantification methods *(Information gathered from Section 1.3 and 2.2.2)*			**Is this parameter usually measured at a typical FeCr furnace?** *(Information gathered from Section 2.2.4)*
Symbol used in tier equations		**Description**	
Tier 1	MPi	Production of ferroalloy i	Yes M
	EFi	Generic emission factor for ferroalloy i	(Generic, provided)
Tier 2	$EF_{reducing\ \ agent,i}$	Emission factor of reducing agent i	(Generic, provided)
Tier 3	$CContent_{reducing\ agent,i}$	Carbon content in reducing agent i	Yes C
Tier 2 and Tier 3	$M_{reducing\ agent,i}$	Mass of reducing agent i	Yes M
	$M_{ore,\ h}$	Mass of ore h	Yes M
	$CContent_{ore,h}$	Carbon content in ore h	No C
	$M_{slag\text{-}forming\ \ material,\ j}$	Mass of slag-forming material j	Yes M
	$CContent_{slag\text{-}forming\ \ material,j}$	Carbon content in flux j	No C
	$M_{product,\ k}$	Mass of product k	Yes M
	$CContent_{product,\ k}$	Carbon content in product k	No C
	$M_{non\text{-}product\ \ outgoing\ \ stream,\ l}$	Mass of slag l	Yes; however calculated, not measured M
	$CContent_{non\text{-}product\ \ outgoing\ \ stream,\ l}$	Carbon content in slag l	No C

Data is available — *Data is available, but not in the correct format* — *Data is not measured* — *"M" – mass measurements* *"C" – composition measurement*

All data required by the equations for quantifying the CO_2 emissions (mass of the input streams, mass of the product streams, and carbon content of all the material streams) has been discussed briefly in Section 2.2.4. The next section (2.2.5) will provide information on the processing, evaluation and conditioning of this data.

2.2.5 Data quality evaluation

Data quality is important and needs to be monitored pro-actively [131]. When evaluating the CO_2 emissions from a FeCr furnace by using tier 1, 2, or 3, a significant amount of data needs to be collected, processed, and analysed. Thorough data evaluation is therefore necessary.

A study done by Booysen [132] provided a data quality evaluation method that was developed to identify any potential errors and abnormalities. This method consists of four steps: the first three steps aim to identify abnormal measurements, whereas the final step identifies abnormal operation. A schematic flow of this method is shown in Figure 2-2.

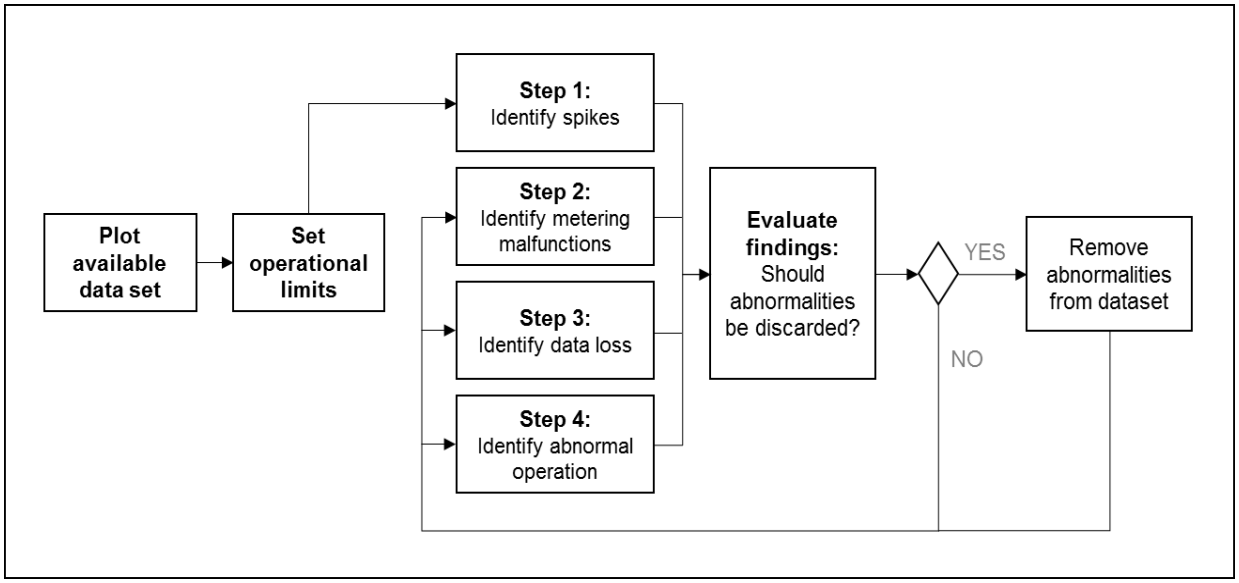


Figure 2-2: Data quality evaluation

Figure 2-3 provides a simplified visualisation of a dataset containing typical measurement abnormalities. The minimum and maximum limits are selected based on the variable being assessed. Steps 1 – 3 are indicated on this figure as follows: data spikes (step 1), faulty data (step 2), and data loss (step 3).

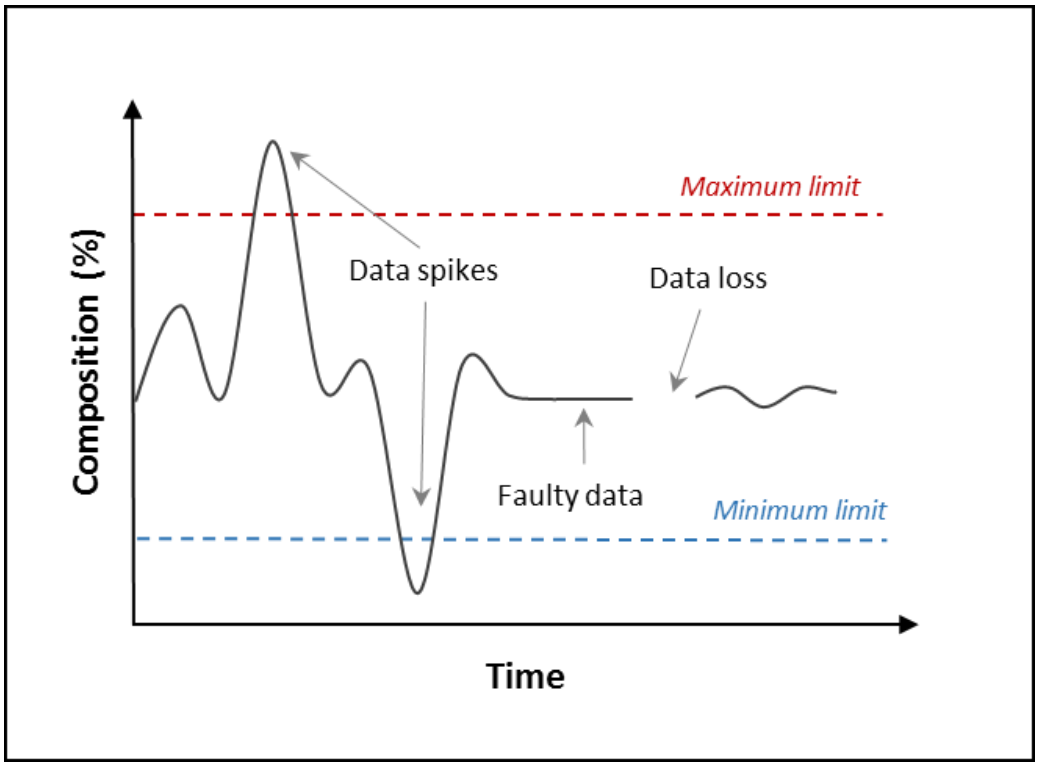


Figure 2-3: Data evaluation – Identifying abnormal measurements

The first step in identifying abnormal measurements in the data evaluation method aims to detect data spikes. Data spikes happen when there is a failure on measurement equipment, or when communication is briefly lost. Even though these tend to happen over short periods of time, their amplitude (very high or very low) can still significantly influence the accuracy of calculations.

The next step is to identify metering malfunctions, which could lead to faulty data being logged. This occurrence is illustrated as a constant value in Figure 2-3, where the last data reading is typically repeated for a number of resolutions, until the malfunction has been resolved. Even though this data will still fall within the operational limits, the results will be influenced by this incorrect, constant value.

Step 3 aims to identify data loss. This can generally be detected where no data has been recorded, as indicated by the blank space in Figure 2-3. The final step of this method aims to identify abnormal system operation. This is illustrated by Figure 2-4.

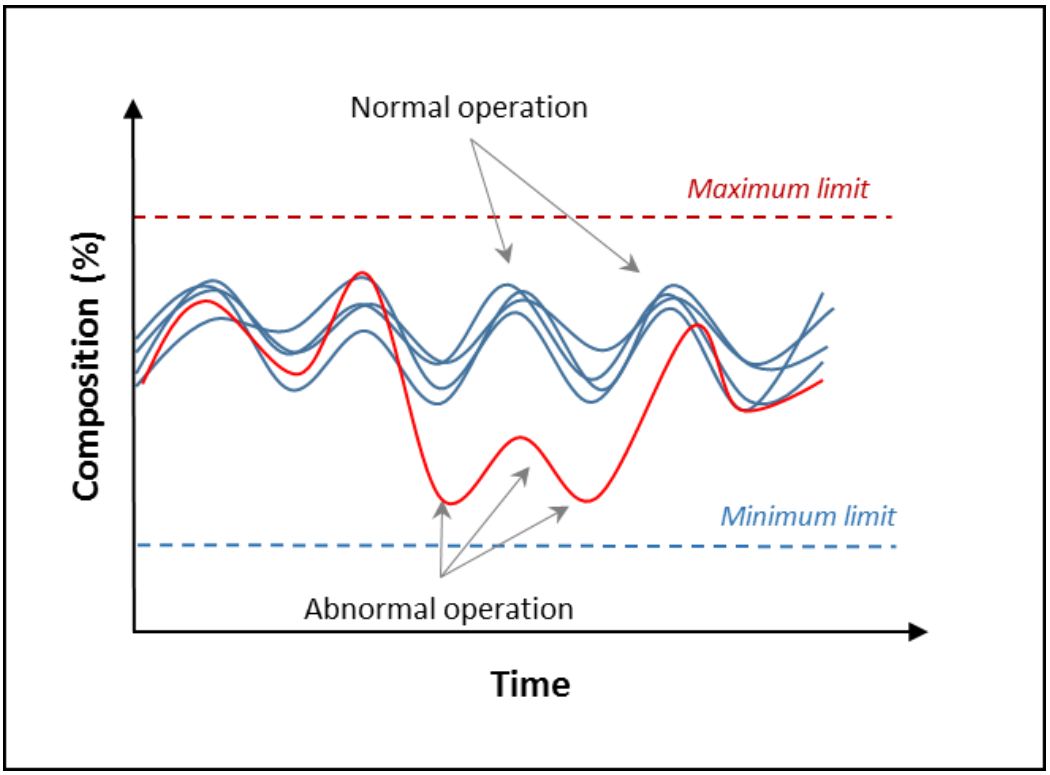


Figure 2-4: Data evaluation – Identifying abnormal operation

In Figure 2-4 there are numerous profiles that follow the same trend, indicating normal operation. The red profile, however, is deemed abnormal, as it differs from the trend. The utmost care should be taken when investigating these results as there is, unfortunately, no fixed rule as to what is defined as "abnormal operation". This step therefore requires a thorough understanding of the process being evaluated.

The aim of the data quality evaluation section is to evaluate a dataset, remove any measurement abnormalities, and identify operational abnormalities. An accurate, high quality dataset is the final outcome of this section.

2.2.6 Research summary and list of assumptions

The literature study provided information on various themes, creating a good knowledge to prepare for practically applying the prescribed CO_2 quantification methods.

Based on all the research done in Section 2.2, a list of assumptions is made in order to do further calculations. This list of assumptions will be used as the first step in the methodology development (Section 2.3):

Table 2-6: List of assumptions

Nr:	Assumption:	Reason for assumption:
1	Ore, reductant, and fluxes enter a FeCr furnace.	Usually the case, according to literature. (Sections 2.2.3 and 2.2.4)
2	FeCr product, slag, and off-gases exit the furnace.	
3	Batching (feed) streams mass is usually measured.	
4	FeCr production is always measured.	
5	Slag production is accurately calculated through a slag to metal ratio.	
6	All data from site is measured, transferred, stored, processed and used correctly.	Data needs to be correct in order to be used in calculations.
7	An annual constant composition is representative enough, and will have no major effect on the final results.	If compositions of feed materials are measured, an unknown buffer capacity (e.g. stockpiles) exists until batched.
		Sometimes the compositions are not available consistently, thus a constant average should be used.
8	Assume carbon content from proximate analyses for reductants (by means of assuming fixed carbon = carbon content).	Usually only proximate analyses are available, not ultimate analyses. *See footnote below (*)*
9	Assume that all raw materials are dried when sampled for analyses, and when entering the furnace	(If there is a pre-heater or dryer present)
10	A 5% error is acceptable.	Data quality evaluation will remove outliers with an error of 5% or higher.

* ***Proximate analysis*** *measures the moisture (M), ash (A), volatile matter (VM) and fixed carbon (FC) content of the coal* [133].

* ***Ultimate analysis*** *measures the carbon (C), hydrogen (H), oxygen (O), nitrogen (N) and sulphur (S) of the coal.* [133].

2.3 Methodology

2.3.1 Preamble

The problem statement in Chapter 1 noted that the process of quantifying the CO_2 emissions from a FeCr furnace is uncertain. Section 2.2 reviewed the relevant literature needed to fully understand the details to comprehensively investigate a FeCr furnace and quantify its CO_2 emissions. The literature findings from Section 2.2 will be used to construct a generic methodology to practically and systematically apply the prescribed methods.

This methodology will be categorised into four divisions, which will be discussed in the following sections. These include listing the assumptions and information required; collecting information, layouts and data; evaluating data quality; and finally, applying the existing methods. This approach is presented in Figure 2-5 (below) and will be discussed in detail in Sections 2.3.2 to 2.3.5.

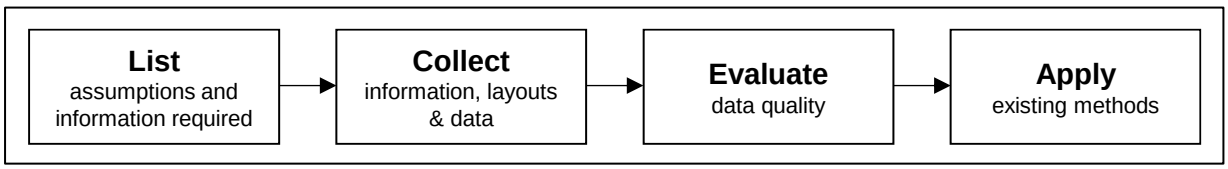


Figure 2-5: Four-step approach to practically apply the prescribed quantification methods

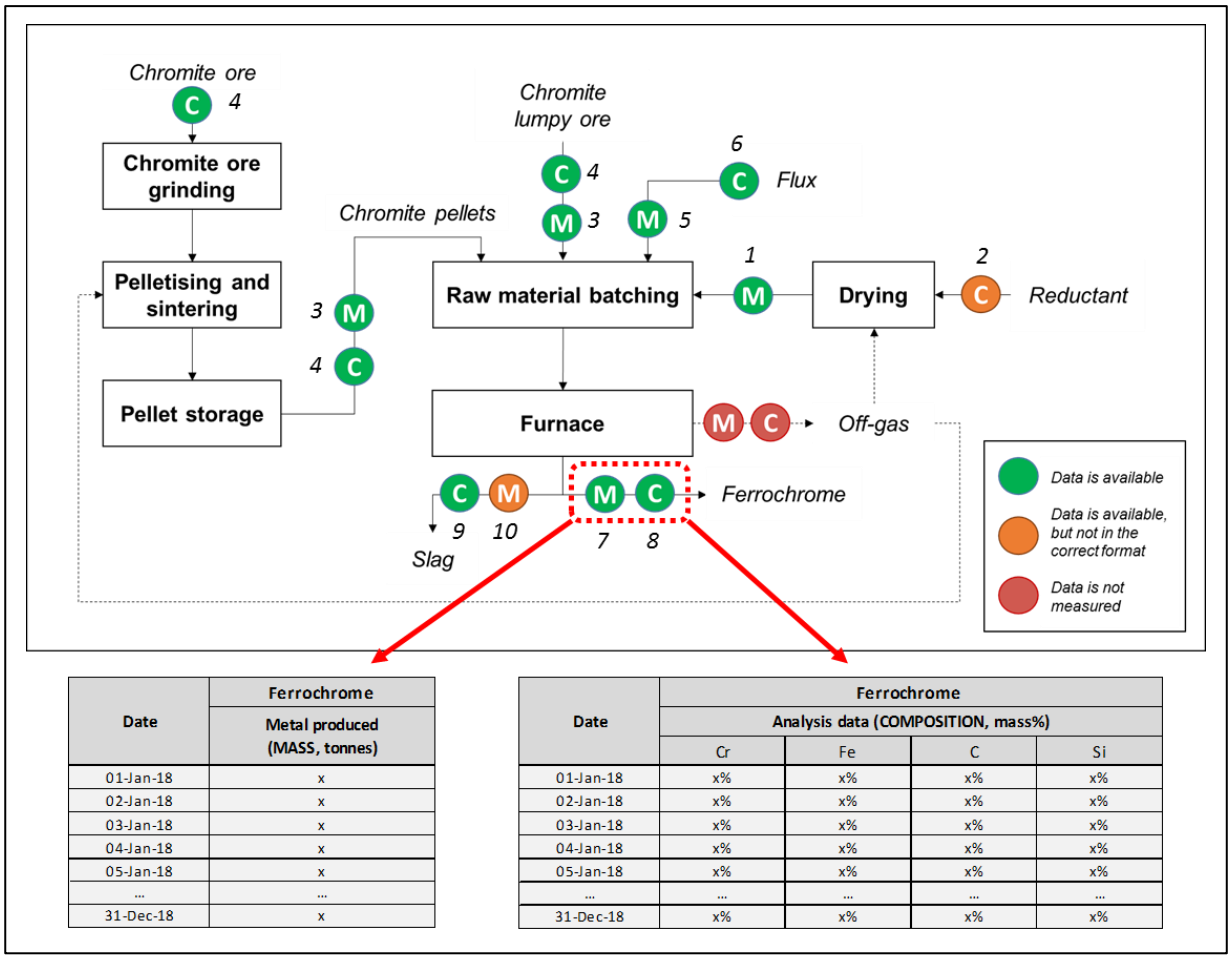
2.3.2 List of assumptions and information required

When listing the assumptions and information required, one can refer back to Table 2-3 and Table 2-6. All sites will require the same information and data to calculate the CO_2 emissions. However, each unique case might have different additions to the list of assumptions.

2.3.3 Collect information, layouts, and data

The next step is to collect all relevant information from the site being evaluated. This includes layouts of the furnace, the relevant points of measurement indicated on layouts, and the corresponding mass and composition data for the evaluation period. Figure 2-6 indicates the outcome of this step.

Note that, for illustration purposes, only data collected for ferrochrome metal production is shown on the layout (mass and composition data). However, the relevant data from all available streams must be collected. Note the labels *1 – 10* on Figure 2-6, which indicate the specific parameters needed for the prescribed methods, as discussed at Figure 2-1.



Date	Ferrochrome
	Metal produced (MASS, tonnes)
01-Jan-18	x
02-Jan-18	x
03-Jan-18	x
04-Jan-18	x
05-Jan-18	x
...	...
31-Dec-18	x

Date	Ferrochrome			
	Analysis data (COMPOSITION, mass%)			
	Cr	Fe	C	Si
01-Jan-18	x%	x%	x%	x%
02-Jan-18	x%	x%	x%	x%
03-Jan-18	x%	x%	x%	x%
04-Jan-18	x%	x%	x%	x%
05-Jan-18	x%	x%	x%	x%
...	...	...	...	...
31-Dec-18	x%	x%	x%	x%

Figure 2-6: Collect information, layouts, and data

The circles on the layout represent points of measure. Green circles indicate that data is available, orange represents available data, but not in the correct format, while red circles indicate that data is not available, or not measured. The "M" symbols refer to mass measurements (by means of weighbridges or weigh bins), whereas the "C" denotes composition analysis sampling. Note that these statuses (colours) are just example illustrations, and that other configurations may also exist.

If data is required for an orange-indicated measurement point (data that is available, but not in the correct format), data needs to be processed to the correct analysis by making use of various methods or assumptions. An example of such a case is when the reductant composition is based on proximate analyses instead of ultimate analyses. The slag mass may also not be available. However, slag-to-metal ratio data can be used to calculate a theoretical slag mass. If data is required from a red-indicated meter, the data cannot be collected and the specific prescribed method can simply not be executed.

2.3.4 Evaluate data quality

A "good" quality dataset is of great importance. It is essential that all data received in the previous step (Section 2.3.3) is a reflection of the truth. The third step of the methodology is the evaluation of the data quality. The method referred to in Section 2.2.5 must be followed for all mass- and composition measurement data, with the aim to "clean" the dataset. This will ensure accurate and representative data. Only then can the data be processed and used in the relevant calculations.

2.3.5 Apply prescribed methods

After the layouts are understood and data has been collected, the "cleaned" dataset must be applied to the prescribed methods: Tier 1, 2, 3. Even though there is no indication of data resolution specifications, the Carbon Tax legislation suggests that CO_2 emissions be reported every six months [25]. Monthly resolution data will thus be used for all calculations. Actual, but fictional, values will be used to clearly illustrate the calculations being done in a practical way.

Tier 1: Production-based emission factors

Tier 1 uses the production mass of FeCr metal, as well as a universal FeCr emission factor to determine the amount of CO_2 emissions. Figure 2-7 shows a practical example of calculating these emissions for one month using tier 1 (Equation 1-3). Assume that this specific FeCr plant consists of a PSP (as seen in Figure 2-6), hence EF*i* = 1.6 tonnes CO_2 / tonnes FeCr produced.

Date	*MP* *(tonnes)* 7	E_{CO_2} *(tonnes)* -
Jan-15	10 000	**16 000**
Feb-15	10 500	**16 800**
Mar-15	9 000	**14 400**
…	…	**…**
Dec-15	…	**…**

$$E_{CO_2} = \sum_i (MP_i \times EF_i)$$

$$= \left(10\,000\ tonnes \times \frac{1.6\ tonnes\ CO_2}{tonnes\ FeCr\ produced}\right)$$

$$= 16\,000\ tonnes\ CO_2$$

Figure 2-7: Example illustration of applying tier 1

Tier 2: Production-based, raw material-specific emission factors

Tier 2 uses the mass and carbon content of all inlet and outlet streams (except for the reducing agent where an EF is used) to calculate the CO_2 emissions. Figure 2-8 shows an illustration where CO_2 emissions are calculated for one month using tier 2 (Equation 1-4). Assume that, for this example, the EF of the reducing agent is 3.2 tonnes CO_2 / tonnes reducing agent used, and the carbon contents of the ore, fluxes, FeCr metal, and slag are 0, 0.2, 0.08 and 0, respectively.

Date	$M_{reducing}$ (tonnes) 1	M_{ore} (tonnes) 3	M_{flux} (tonnes) 5	$M_{product}$ (tonnes) 7	M_{slag} (tonnes) 9	E_{CO2} (tonnes) -
Jan-15	4 000	20 000	1 000	10 000	12 000	**10 600**
Feb-15	…	…	…	…	…	…
Mar-15	…	…	…	…	…	…
…	…	…	…	…	…	…
Dec-15	…	…	…	…	…	…

$$E_{CO_2} = \sum_i (M_{reducing\ agent} \times EF_{reducing\ agent}) + \sum_h (M_{ore} \times Ccontent_{ore}) \times \frac{44}{12} + \sum_j \left(M_{flux} \times Ccontent_{flux}\right) \times \frac{44}{12} - \sum_k (M_{product} \times Ccontent_{product}) \times \frac{44}{12} - \sum_l (M_{slag} \times Ccontent_{slag}) \times \frac{44}{12}$$

$$E_{CO_2} = (4\,000 \times 3.2) + (20\,000 \times 0) \times 44/12 + (1\,000 \times 0.2) \times 44/12 - (10\,000 \times 0.08) \times 44/12 - (12\,000 \times 0) = \mathbf{10\,600\ tonnes\ CO_2}$$

Figure 2-8: Example illustration of applying tier 2

Tier 3: Calculations based on amounts and analyses of reducing agents

Tier 3 is similar to tier 2. However, site-specific compositions must be used. The carbon content of reducing agents is also to be used instead of generic emission factors. Figure 2-9 shows how tier 3 (Equation 1-5) is used to calculate the CO_2 emissions from the specific furnace. Assume that the C-content of the reductant is 0.85 [125], whereas the other contents remain unchanged.

Date	$M_{reducing}$ (tonnes) 1	M_{ore} (tonnes) 3	M_{flux} (tonnes) 5	$M_{product}$ (tonnes) 7	M_{slag} (tonnes) 9	E_{CO2} (tonnes) -
Jan-15	4 000	20 000	1 000	10 000	12 000	**10 267**
Feb-15	…	…	…	…	…	…
Mar-15	…	…	…	…	…	…
…	…	…	…	…	…	…
Dec-15	…	…	…	…	…	…

$$E_{CO_2} = \sum_i (M_{reducing\ agent} \times Ccontent_{reducing\ agent}) \times \frac{44}{12} + \sum_h (M_{ore} \times Ccontent_{ore}) \times \frac{44}{12} + \sum_j \left(M_{flux} \times Ccontent_{flux}\right) \times \frac{44}{12} - \sum_k (M_{product} \times Ccontent_{product}) \times \frac{44}{12} - \sum_l (M_{slag} \times Ccontent_{slag}) \times \frac{44}{12}$$

$$E_{CO_2} = (4\,000 \times 0.85) \times 44/12 + (20\,000 \times 0) \times 44/12 + (1\,000 \times 0.2) \times 44/12 - (10\,000 \times 0.08) \times 44/12 - (12\,000 \times 0) = \mathbf{10\,267\ tonnes\ CO_2}$$

Figure 2-9: Example illustration of applying tier 3

2.3.6 Methodology summary

The process of quantifying the CO_2 emissions from a FeCr furnace is uncertain. A generic approach was therefore constructed to practically and thoroughly apply the prescribed quantification methods. The four steps in this approach include listing assumptions and information required (2.3.2), collecting information, layouts and data (2.3.3), evaluating data quality (2.3.4), and finally, applying the prescribed methods (2.3.5). The strategy that was developed in Section 2.3 is based on the research done in Section 2.2, and is illustrated in Figure 2-10 below:

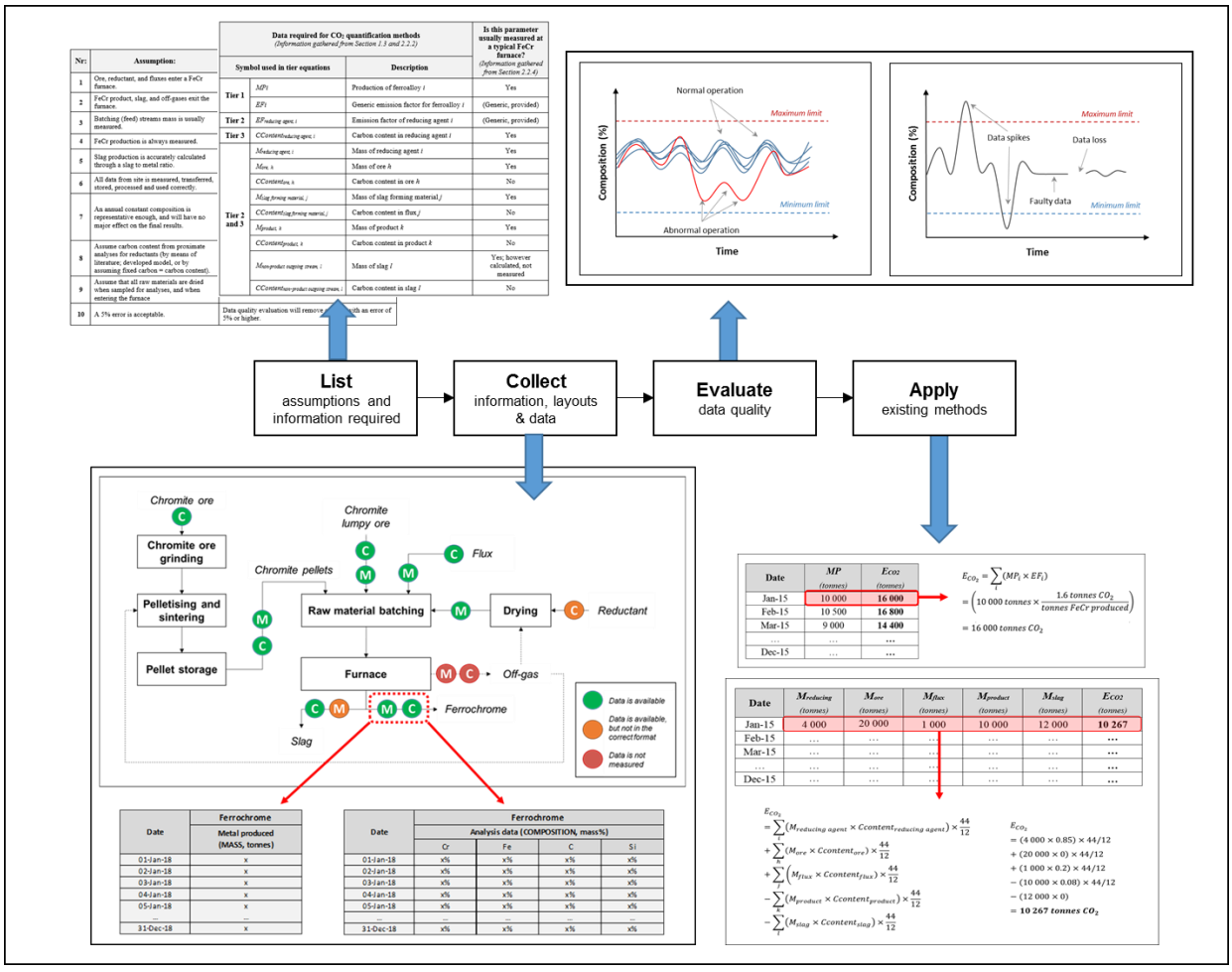


Figure 2-10: Four-step approach to practically apply the prescribed quantification methods

In the next section, this approach will be used and applied to a real-life FeCr furnace (case studies). These case studies will illustrate how each of the four steps (*List*, *Collect*, *Evaluate* and *Apply*) is essential to determine the best possible results. This will be done by highlighting the potential constraints that may occur during the practical application of the prescribed methods.

2.4 Case studies: Results and discussion

2.4.1 Preamble

The methodology provided an approach to follow when calculating the CO_2 emissions from a FeCr furnace based on the prescribed methods. It was found that the equations are relatively easy to apply if the correct information and data is known. Three detailed case studies (CS) will be used to highlight the importance of certain areas in the methodology developed in Section 2.3, by introducing potential constraints that may occur during the practical application of the prescribed methods. These include illustrating the importance of: CS1) efficient collection of layouts and information; CS2) choosing the most relevant emission factors; and CS3) data quality.

2.4.2 Case study background

Information, the relevant points of measure and the corresponding mass and composition data over a one-year evaluation period have been collected for furnace X. This is shown in Figure 2-11.

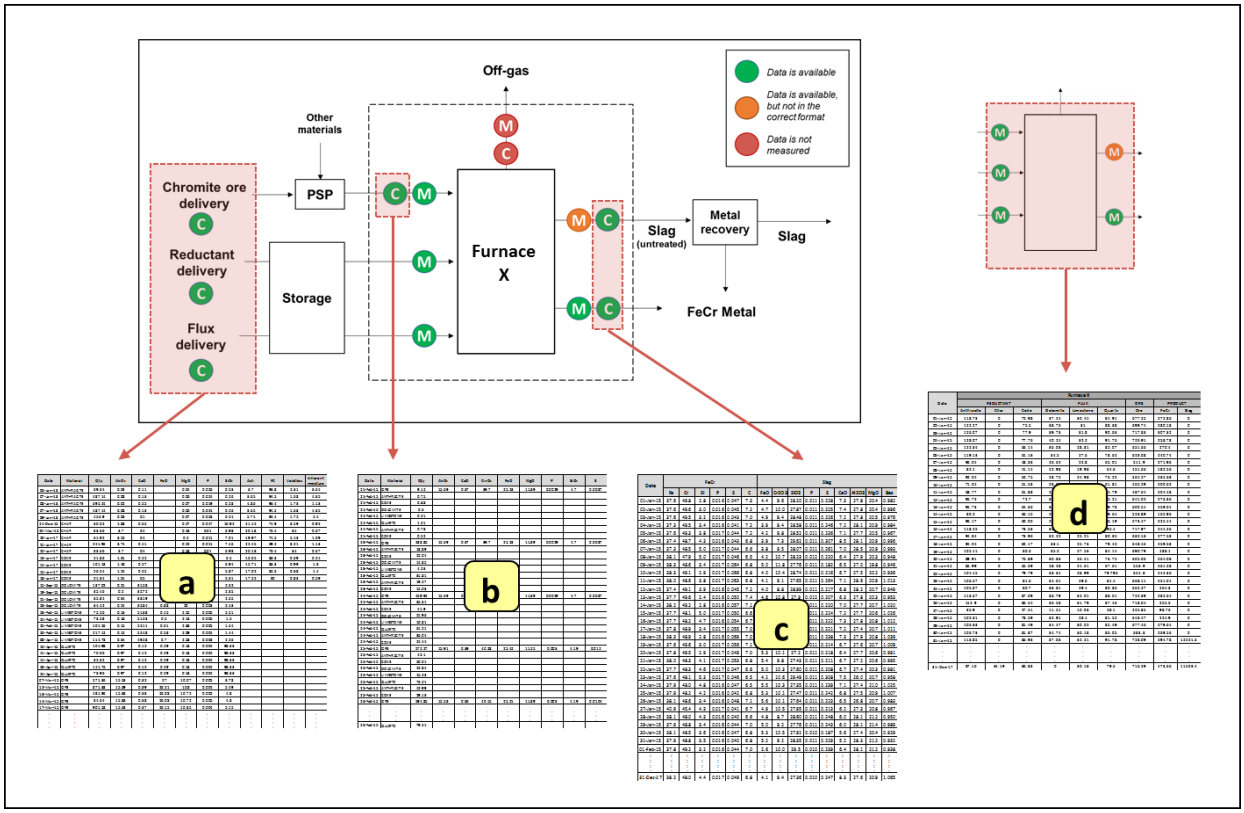


Figure 2-11: Collect information, layouts, and data

Chrome ore, reductant (anthracite, char, and coke), and fluxes (dolomite, limestone, and quartz) are sampled on delivery (dataset "a"). Chromite ore is pelletised (PSP), and sampled again before

batching (dataset "b"). The composition of the FeCr metal and slag is also determined when exiting the furnace (dataset "c"). The mass of all raw materials are determined in weigh bins right before batching, whereas the FeCr metal and slag mass are measured at weighbridges (dataset "d").

These four datasets have been collected so as to be evaluated throughout the next step. Note that the slag mass meter is indicated in orange. This is due to the slag mass only being logged per month, when the rest of the data is in daily resolution. Thus, all data will be converted to monthly resolution when processing and calculations commence. The time delay that may occur between mass and composition measurements is uncertain. All compositions will therefore be averaged to a constant annual value, in order to compensate for any possible storage capacities.

The case studies that follow will not only quantify the CO_2 emissions by means of a specific prescribed method, but will focus on highlighting the potential constraints that may exist, and quantify the effect of this constraint.

2.4.3 Case study 1: Collection of information and layouts

Case study 1 will illustrate the importance of obtaining the correct information and layouts from site. As seen in Figure 2-11, there is a PSP present on site, which prepares the raw materials before being fed to the furnace. However, since the PSP has been out of order for the period to be evaluated, the raw materials were not pelletised or sintered.

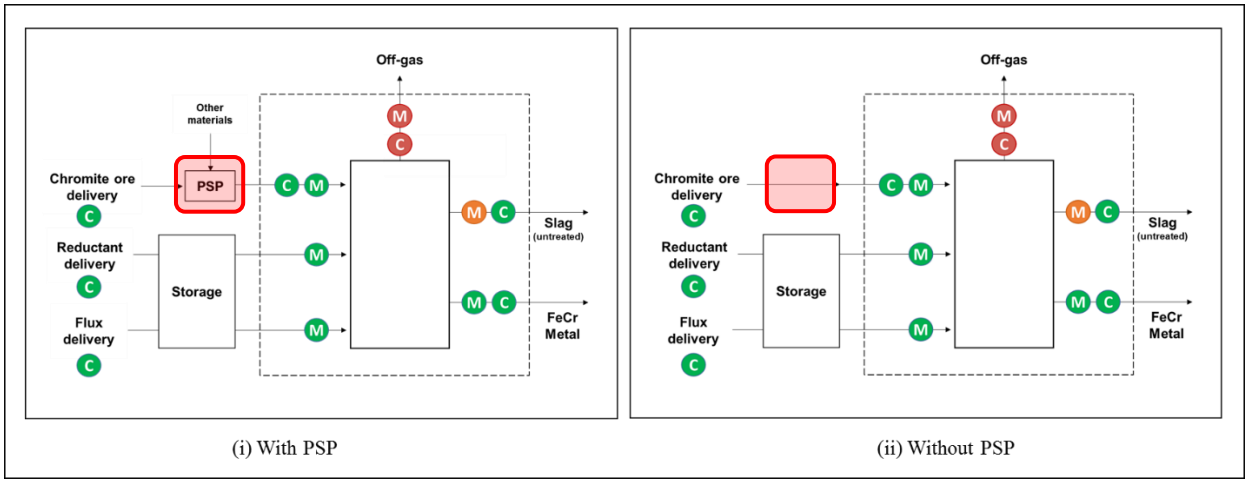


Figure 2-12: Incorrect (i) and correct (ii) layout of furnace X

Tier 1 (Equation 1-3) will be used to test the effect of having the (in)correct information of the site evaluated. The CO_2 emissions will thus be calculated based on the first (incorrect) information: PSP present (i), and with the eventually correct information: no PSP present (ii).

(i) $E_{CO_2} = \sum_i (MP_i \times EF_i) = E_{CO_2} = \sum_i (MP_i \times \mathbf{1.6})$

(ii) $E_{CO_2} = \sum_i (MP_i \times EF_i) = E_{CO_2} = \sum_i (MP_i \times \mathbf{1.3})$

The calculations were done for each scenario (according to Figure 2-7) and the results were aggregated for one year. This is shown in Figure 2-13 below.

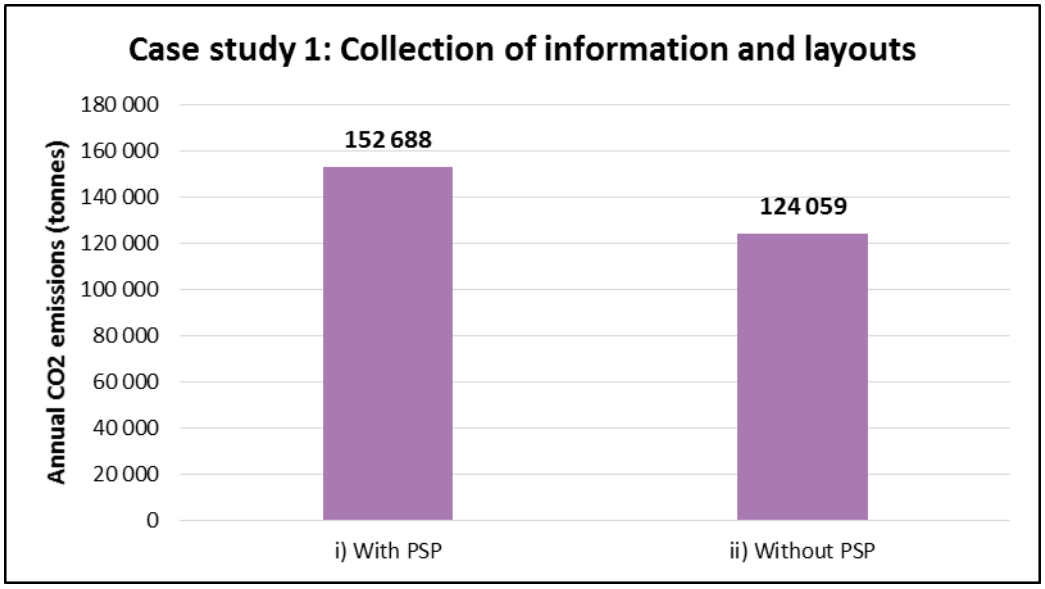


Figure 2-13: Case study 1 results

If the incorrect information or layout is used to calculate the CO_2 emissions, it will result in an error of 18.8% (difference between 152 688 tonnes and 124 059 tonnes). The detailed calculations and results can be seen in Appendix D. Fortunately, the absence of the PSP will not have an effect on any other calculations other than tier 1, as explained and illustrated above.

2.4.4 Case study 2: The effect of different emission factors

Based on Table 2-2 (providing information on the generic emission factors [EFs] for reducing agents) in Section 2.2.6, it is seen that these EFs can vary somewhat. It is possible that the EF chosen may not necessarily be accurate for the specific reductant applicable. Case study 2 will therefore investigate the importance of using the most relevant EFs.

Tier 2 (Equation 1-4) will be used to test the effect of choosing the less relevant EFs for the specific reductants used. The CO_2 emissions will thus be calculated based on the EFs from reference A, as stipulated in Table 2-2 (i), as well as with the EFs from reference B (ii). The EFs used is listed below (all EF values in tonnes CO_2 / tonne reducing agent):

(i) Coal = **2.96**, coke = **3.21**, anthracite = **2.602** *(assumed; reference A does not include anthracite)*

(ii) Coal = **2.325**, coke = **2.819**, anthracite = **2.602**

The calculations were done for each scenario (according to Figure 2-8) and the results were aggregated for one year. This is shown in Figure 2-15 below.

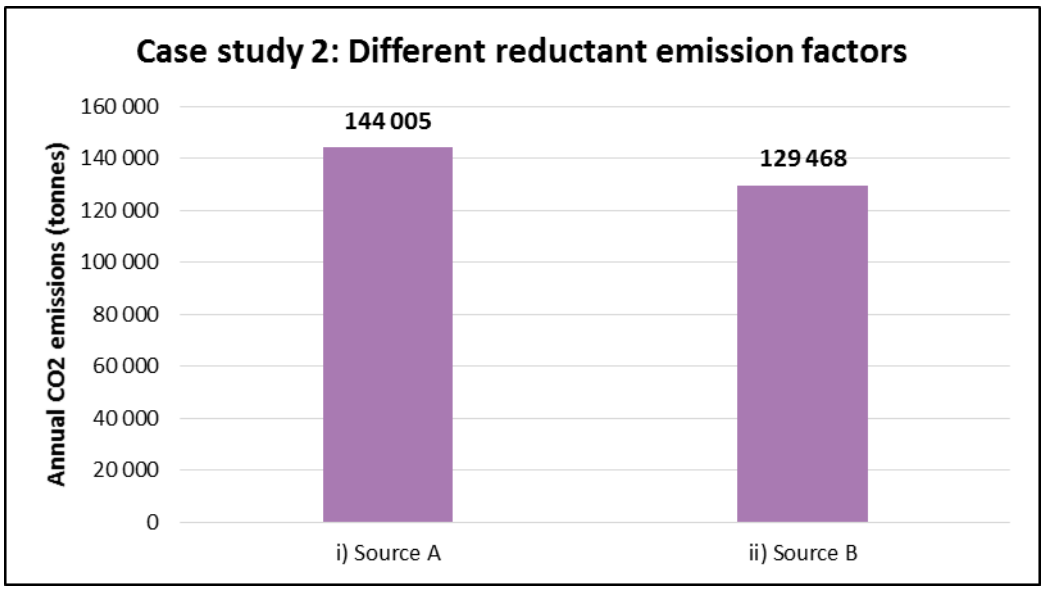


Figure 2-14: Case study 2 results

If the incorrect EFs are used to calculate the CO_2 emissions, it can result in an error of 10.1%. The detailed calculations and results can be seen in Appendix D.

2.4.5 Case study 3: The effect of data quality

Case study 3 will be used to illustrate the importance of having a good quality dataset, and implementing a thorough data quality assessment. The raw datasets as received in Figure 2-11 (datasets "a", "b", "c", and "d") must be evaluated based on the method discussed in Section 2.2.5. Figure 2-15 illustrates one of the datasets before (i) and after (ii) the dataset has been cleaned.

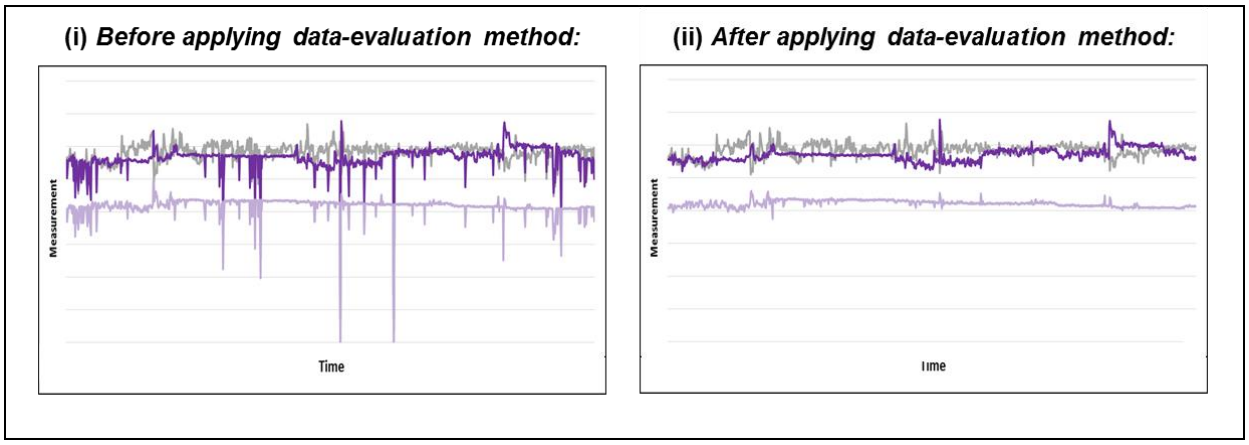


Figure 2-15: Data quality evaluation

Any abnormal measurements within the data have been identified, investigated and removed, if necessary. Annual shutdowns were detected (where furnace was shut down for a month or two). However, data was not removed, since this is not an abnormal operational occurrence. Consequently, after applying the method of data quality evaluation, all datasets are of high quality and can be used in further calculations.

Tier 3 (Equation 1-5) will be used to test the effect of thorough data quality evaluation. The CO_2 emissions will thus be calculated based on the original data received (i), and with the "cleaned" dataset (ii). The calculations were done for each scenario (according to Figure 2-9) and the results were aggregated for one year. This is shown in Figure 2-16 below.

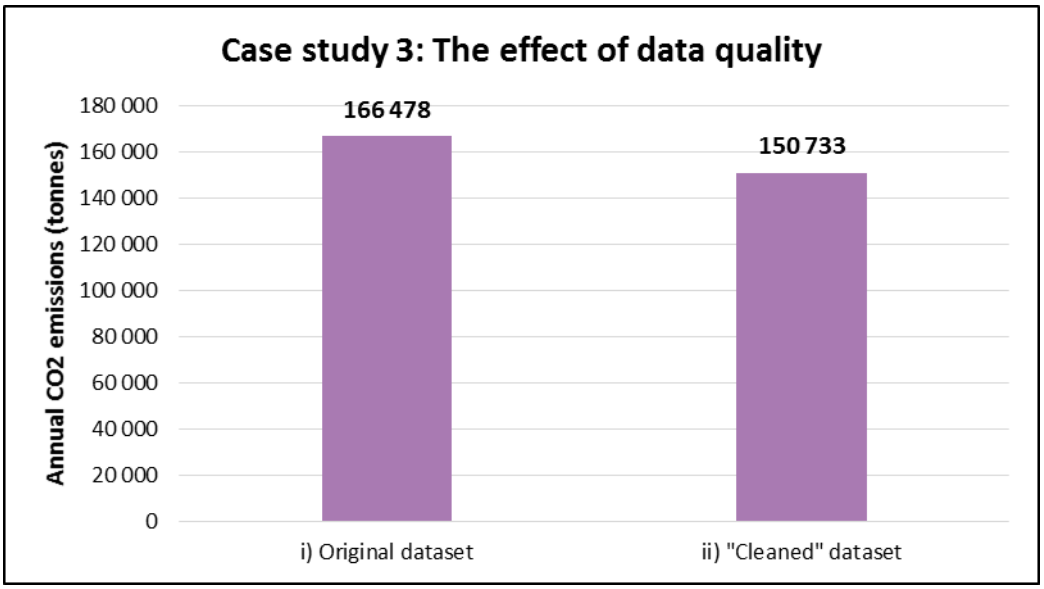


Figure 2-16: Case study 3 results

If all datasets (used to calculate the CO_2 emissions) are not evaluated and "cleaned" to a sufficient quality, it may result in a significant error, which is calculated as 9.5% for this specific case study. The detailed calculations and results can be seen in Appendix D. This error can vary significantly, depending on the initial quality of the data received.

2.4.6 Case study summary

Three case studies were done to highlight the significance of certain areas in the methodology. The results of these case studies are provided in Table 2-7:

Table 2-7: Case study results summary

Case study	Section	Aim	Quantified effect	Tier used to illustrate the case study
CS 1	2.4.3	Evaluate the effect of having the correct information and layouts of the plant	18.8%	Tier 1
CS 2	2.4.4	Evaluate the effect of using the correct emission factors	10.1%	Tier 2
CS 3	2.4.5	Evaluate the effect of data quality investigation and conditioning	9.5%	Tier 3

From this table it is evident that less accurate results may be obtained if the correct procedure is not followed. It can therefore be stated that the methodology developed in Section 2.3 is sufficient, as it provides a good and systematic way to approach the practical quantification of CO_2 emissions from FeCr furnaces.

After highlighting the importance of each step in the methodology, and quantifying the impact of having the "incorrect" information, the final correct results can be illustrated. Tier 1 is calculated by using the correct EF, i.e. not taking a PSP into account (CS1, result ii). Tier 2 is calculated by taking the average of results from source A and source B (CS2, results i and ii), since the correct EF is not known. The tier 3 calculation was done with the "cleaned" dataset (CS3, result ii). The final results from the prescribed methods are illustrated in Figure 2-17.

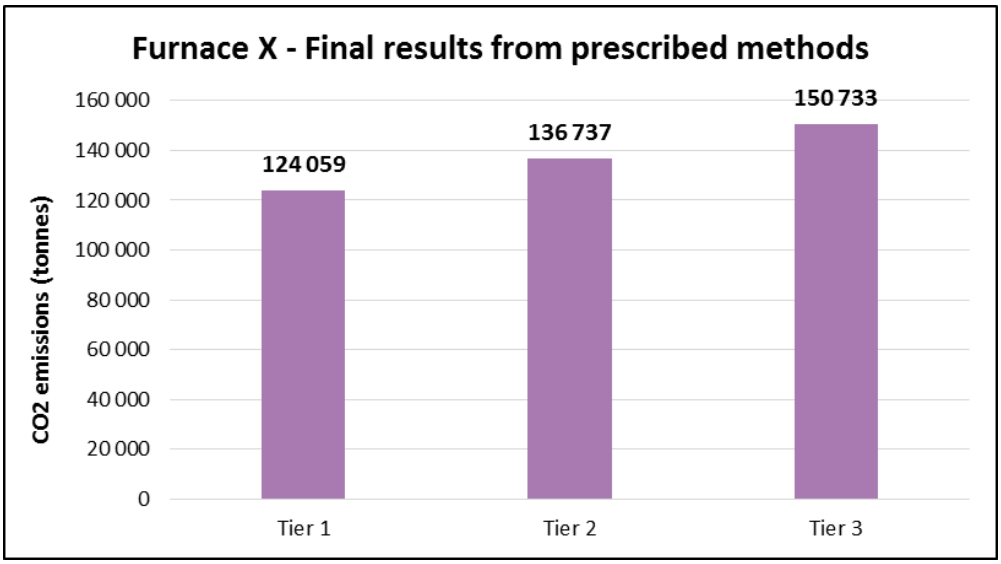


Figure 2-17: Final results from prescribed methods (Furnace X)

This section used one furnace (Furnace X) for all three case studies. In addition to this, 16 other furnaces were also investigated, and similar case studies were done. Table 2-8 provides a summary of the results for all 17 furnaces, showing an average of the quantified effect for each potential/induced constraint (as with Table 2-7). More detail regarding these results can be seen in Appendix E.

Table 2-8: Average of 17 furnaces case study results summary

Case study	Aim	Quantified effect	Tier used to illustrate the case study
CS 1	Evaluate the effect of having the correct information and layouts of the plant	18.8%	Tier 1
CS 2	Evaluate the effect of using the correct emission factors	11.2%	Tier 2
CS 3	Evaluate the effect of data quality investigation and conditioning	8.9%	Tier 3

This table represents the average quantified effects of the different constraints for the 17 furnaces investigated. These results confirm that less accurate results may be obtained if the correct procedure is not followed. The methodology developed in Section 2.3 is therefore verified as sufficient, as it provides a good and systematic way to approach the practical quantification of CO_2 emissions from FeCr furnaces.

2.5 Conclusion

No sufficient practical examples of applying the prescribed CO_2 emission calculations could be found in literature. The need for illustrating the practical application of these methods was, however, addressed in this chapter. It provided the relevant literature on emission calculations for carbon tax purposes, the FeCr industry, and the evaluation of data quality. A methodology was then developed to be used when applying the prescribed methods. Case studies were used to practically apply these calculation methods, and illustrate the significance of certain areas in the methodology. It was found that, without the methodology developed, one is likely to obtain less accurate results (possible errors of 8.9% - 18.8%) when performing the prescribed calculations.

The three calculation methods (tier 1, 2 and 3) are the only ones available from literature. Even though these are relatively simple to apply, it is still uncertain as to if the final results are accurate. The next chapter will therefore explore the idea of refining these methods into a more complex, yet accurate approach. The construction of various mass balances will be used to test this idea.

3. REFINEMENT OF PRESCRIBED METHODS

3.1 Introduction

Furnaces used for ferrochrome production are complex systems. There are a significant number of inlet and outlet streams with various parameters. However, some of these parameters are not always measured, which can limit the application of some of the prescribed methods to quantify the CO_2 emissions from the furnace. Currently there are three methods for quantifying the CO_2 emissions from FeCr production. However, from Section 1.3 it was found that these methods are not necessarily equally accurate and may also produce results that vary significantly from one another (Section 2.4). Focus area 2 was identified to evaluate the possibility of improving the current methods.

As a result, there is a need to determine whether it is possible to refine these prescribed methods into a more complex, yet accurate approach. Since tier 3 is the most detailed method and follows a basic mass balance approach, this tier will be investigated even further and applied practically. By linking the available data and additional information together with data analytics, estimates of the unknown streams can possibly be found. Tier 3 uses mass and composition measurements for conducting a mass balance on a FeCr furnace in order to determine the CO_2 emissions. The formula used is given as a repeat of Equation 1-5:

$$E_{CO_2} = \sum_i \left(M_{reducing\ agent,i} \times CContent_{reducing\ agent,i}\right) \times \frac{44}{12} + \sum_h \left(M_{ore,h} \times Ccontent_{ore,h}\right) \times \frac{44}{12} + \sum_j \left(M_{slag-forming\ material,j} \times Ccontent_{slag-forming\ material,j}\right) \times \frac{44}{12} - \sum_k \left(M_{product,k} \times Ccontent_{product,k}\right) \times \frac{44}{12} - \sum_l \left(M_{non-product\ outgoing\ stream,l} \times Ccontent_{non-product\ outgoing\ stream,l}\right) \times \frac{44}{12}$$

The problem is that all of these compositions and mass measurements are not necessarily always measured, which makes it difficult to apply the formula. Mass balances can be used to predict mass and compositions of unmeasured streams [26, 121]. This chapter will therefore use the construction of mass balances to explore the idea of refining the prescribed methods (tier 3). The literature study and methodology, describing the steps when constructing a mass balance, is presented in Section 3.2 and 3.3, respectively. Case studies are used to verify the methodology and illustrate a refined way to calculate FeCr CO_2 emissions.

3.2 Literature study

3.2.1 Preamble

The literature study will provide information from which the methodology in Section 3.3 will be developed. The elements present within the streams entering and exiting a FeCr furnace will be rehashed in Section 3.2.2. A brief discussion of relevant statistical information will then be given in Section 3.2.3, while Section 3.2.4 will provide background information on mass balances and the construction thereof. The literature study will be concluded in Section 3.2.5. An illustration of the literature study section is given in Figure 3-1.

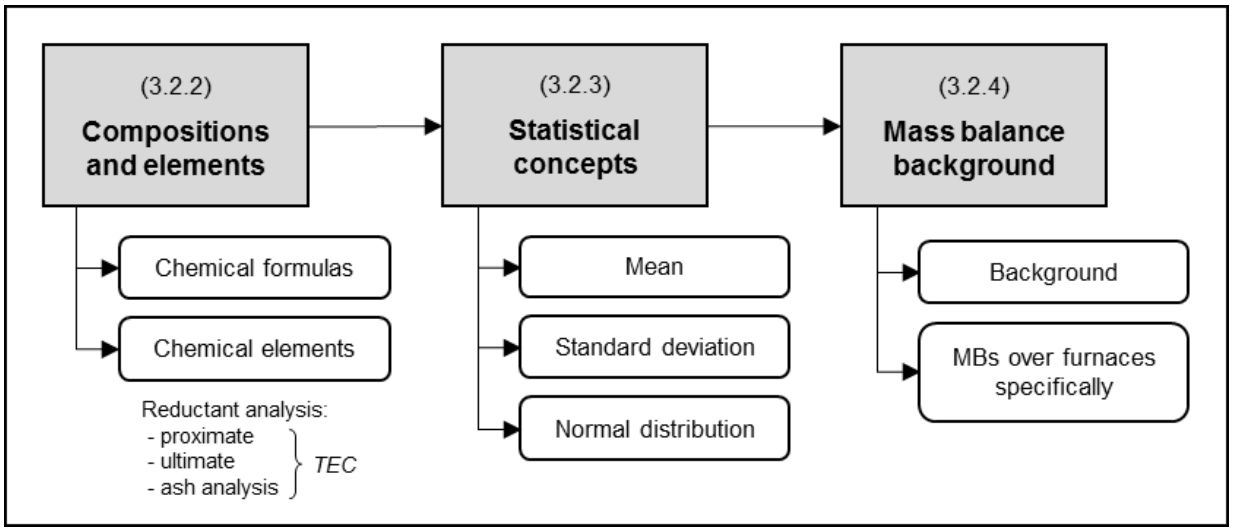


Figure 3-1: Illustration of literature study conduction (Section 3.2)

3.2.2 Compositions and elements present

Various reactions take place in a FeCr furnace which cause the FeCr product to be formed. The most significant reactions include the following [3, 13, 14, 50]:

$Cr_2O_3 + 3C \rightarrow 2Cr + 3CO$	*Equation 3-1: Reduction of chromium oxide*
$FeO + C \rightarrow Fe + CO$	*Equation 3-2: Reduction of iron oxide*
$SiO_2 + 2C \rightarrow Si + 2CO$	*Equation 3-3: Reduction of silicon dioxide*
$H_2O + C \rightarrow H_2 + CO$	*Equation 3-4: Water gas equilibrium reaction*
$CO_2 + C \rightarrow 2CO$	*Equation 3-5: Boudouard reaction*
$CaCO_3 \rightarrow CaO + CO_2$	*Equation 3-6: Decomposition of calcium carbonate*

From these reactions it can be assumed that the prominent elements present in the FeCr furnace are the following: Fe (iron), Cr (chrome), Si (silicon), C (carbon), O (oxygen), H (hydrogen), and Ca (calcium).

Section 2.2.4 briefly discussed the compositions of all streams at a general FeCr furnace. The typical compositions of inlet and outlet streams were converted to element-based compositions by using the molecular weight of each formula and element (Appendix B: Equation B-1 and Equation B-2). Table 2-4 only provided the typical carbon content of each material (which was required by the prescribed CO_2 emission quantification methods).

Since mass balances of all elements entering and exiting a FeCr furnace will be investigated in this chapter, it is important to know the total composition (all elements) of the streams. Table 3-1 therefore provides an updated version of Table 2-4, and gives the total mass composition for streams entering and exiting a FeCr furnace (element-based) [7, 14, 15, 123, 124, 125, 126, 127, 128, 129]:

Table 3-1: Typical compositions for all streams of a FeCr furnace (element-based)

Material	Chemical elements										
	Fe	**Cr**	**Si**	**C**	**Al**	**O**	**Ca**	**Mg**	**H**	**N**	**S**
Cr ore	17.5%	34.2%	2.3%	-	5.2%	34.6%	0.7%	5.4%	-	-	-
Anthracite	-	-	-	88.9%	-	2.3%	-	-	3.4%	1.6%	0.8%
Char	-	-	-	77.8%	-	21.1%	-	-	0.3%	0.7%	-
Coke	-	-	-	89.0%	-	-	-	-	3.6%	1.6%	5.0%
Dolomite	-	-	0%	13%	-	52%	22%	13%	-	-	-
Limestone	-	-	0%	12%	-	48%	40%	0%	-	-	-
Quartz	-	-	47%	-	-	53%	0%	0%	-	-	-
Burnt lime	-	-	0%	-	-	29%	71%	0%	-	-	-
FeCr met	33.8%	56.7%	2.3%	7.2%	-	-	-	-	-	-	-
Slag	8.3%	12.7%	10.8%	-	12.8%	41.3%	2.1%	11.9%	-	-	-
Off-gas	-	-	-	28 - 47%	-	44 - 74%	-	-	0.2 - 1%	2 - 7%	-

**Off-gas composition was converted from volume to mass % by Equation B-5 in Appendix B.*

The theoretical elements from the reactions within the furnace (Equation 3-1 to Equation 3-6) are confirmed by elements present in the streams (Table 3-1). Thus, the typical elements present within the FeCr furnace are the following: Fe (iron), Cr (chrome), Si (silicon), C (carbon), Al (aluminium), O (oxygen), Ca (calcium), Mg (magnesium), H (hydrogen), N (nitrogen) and S (sulphur). The compositional values from Table 3-1, together with mass measurements, may be used in mass balance calculations if no composition data is available from site.

Reductant analyses

The anthracite, char and coke analyses from Table 3-1 were obtained by using the ultimate analysis of these reductants (or coals) from literature. It is, however, confirmed that an ultimate analysis is done on a dry-ash-free (d.a.f.) basis, meaning that the analysis does not account for the ash or moisture within the coals [134, 135]. It therefore only includes the influence of volatiles and fixed carbon. The ultimate analysis (%C, %H, %O, %N, %S), together with the percentage ash and moisture from the proximate analysis, forms a total of 100%, expressed as a mass percentage.

Since the ultimate analysis does not account for all the elements present in the coal (not representative of entire coal batch entering the furnace), it cannot be used when performing an elemental mass balance over a furnace. According to industry experts[4], it is also not possible to determine the elemental composition from the proximate analysis, unless more in-depth knowledge about the coals is available.

Data collected from the Coal and Mineral Services division [136] includes coal samples from across the country from different provinces and coal fields (Table C-1). Three types of analyses, amongst others, were performed on these coals, namely: 1) proximate analysis (fixed carbon, volatile matter, ash and moisture); 2) ultimate analysis (C, H, O, N and S); and 3) ash analysis (SiO_2, Al_2O_3, Fe_2O_3, P_2O_5, TiO_2, CaO, MgO, K_2O, Na_2O, SO_3).

In order to estimate the total elemental composition (TEC) of coal, all three analyses could possibly be used together to develop an approach to estimate this composition. Equation 3-7 shows the assumed formula to determine the content of a certain element (X^*) within the coal:

$$X^* = X_{ultimate} + X_{moisture} + X_{ash}$$

Equation 3-7: Determining the total content of element X in coal

Where:

X^* = Total amount of element X in a certain raw coal, in percentage (%)

$X_{ultimate}$ = Amount of X present within the fixed carbon and volatiles of a certain raw coal (obtained by the ultimate analysis), in percentage (%)

$X_{moisture}$ = Amount of X present within the moisture of a certain raw coal, in percentage (%)

X_{ash} = Amount of X present within the ash of a certain raw coal, in percentage (%)

[4] Rosemary Falcon - Personal correspondence (27 Jul 2018)

Equation 3-7 is also illustrated by Figure 3-2:

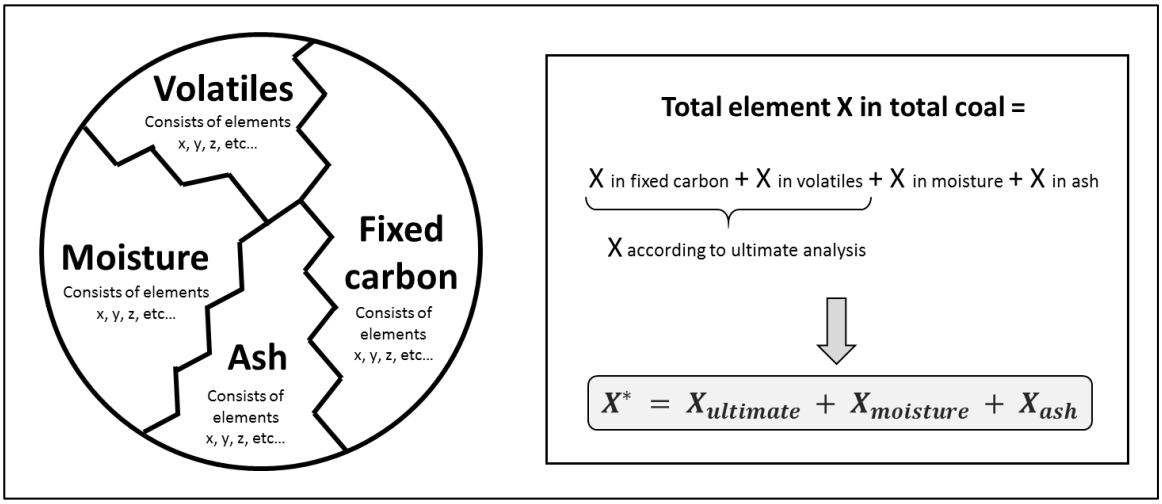


Figure 3-2: Determining the total content of element X in coal

Each "part" of the coal – fixed carbon, volatile matter, moisture and ash (obtained by proximate analysis) – consists of different elements (x, y, z, etc.). All the "X" elements in each part of the coal must be added to determine the total number of "X" elements within the coal. The elemental analysis of the fixed carbon (FC) and volatile matter (VM) is given by the ultimate analysis [134, 135]. The elemental analysis of the moisture is assumed to be 11.2% H and 88.8% O (according to the molar weights of the elements present; assuming that moisture is pure H_2O – see Table C-6), while the elemental analysis of the ash is given by the ash analysis [137].

It should be noted, however, that the ash analysis is done in the presence of excess oxygen and other elements (after the moisture, volatiles and fixed carbon have been driven off), which is not necessarily present in the raw ash of the coal [138]. The elements from the ash analyses (Si, Al, Fe, P, Ti, Ca, Mg, K, Na, S) are expressed as oxides, but may initially exist as a different compound in the raw coal ash, e.g. Fe may exist as FeS_2 (pyrite), but is expressed as SiO_2 and Fe_2O_3 in the ash analysis. The elemental composition of the raw ash can therefore unfortunately not be determined accurately by the ash analysis.

Due to this limitation, the elements from the ash analysis will be regarded as "trace elements". Depending on the magnitude of the ash content of the coal, these assumptions may result in less accurate estimations when the mass balances are constructed. A detailed description of the development of this approach is, however, given in Appendix C.

The elements from the ultimate analysis will be adjusted where applicable (to account for moisture). Equation 3-8 to Equation 3-13 illustrate the estimation of the total elemental

composition (excluding the ash, which is assumed to consist of 100% trace elements) of coal concerning specific elements present in the volatiles, fixed carbon and moisture: C, H, O, N, S.

$$\%C^* = \%C_{ult}$$ *Equation 3-8: TEC of coal (C)*

$$\%H^* = \%H_{ult} + \%Moisture_{prox} \times 0.112$$ *Equation 3-9: TEC of coal (H)*

$$\%O^* = \%O_{ult} + \%Moisture_{prox} \times 0.889$$ *Equation 3-10: TEC of coal (O)*

$$\%N^* = \%N_{ult}$$ *Equation 3-11: TEC of coal (N)*

$$\%S^* = \%S_{ult}$$ *Equation 3-12: TEC of coal (S)*

$$\%Trace^* = \%Ash_{prox}$$ *Equation 3-13: TEC of coal (trace)*

Where "*" refers to the elements from the newly-developed approach (total elemental composition [TEC] analysis) and "Trace" refers to all elements present from the ash analysis (Si, Al, Fe, P, Ti, Ca, Mg, K, Na). Subscripts "*ult*", "*prox*" and "*ash*" refer to the three types of analyses from where the composition values can be found. Note that the parameters $\%C_{ult}$, $\%H_{ult}$, $\%O_{ult}$, $\%N_{ult}$ and $\%S_{ult}$ must first be converted to add to a total of $[100\% - ash - moisture]$, in order for the final calculated TEC elements (*) to be: $\%C^* + \%H^* + \%O^* + \%N^* + \%S^* + \%Trace^* = 100\%$. Table C-2 (Appendix C) provides the final results of the approach applied.

After a detailed evaluation of the composition of coal, it is evident that the typical elements present within the FeCr furnace are the following: Fe (iron), Cr (chrome), Si (silicon), C (carbon), Al (aluminium), O (oxygen), Ca (calcium), Mg (magnesium), H (hydrogen), N (nitrogen) and S (sulphur), as well as some trace elements in the form of P (phosphorus), Ti (titanium), K (potassium) and Na (sodium). This section provided information on compositions and elements within the FeCr process, and is illustrated in Figure 3-3 (highlighted yellow blocks).

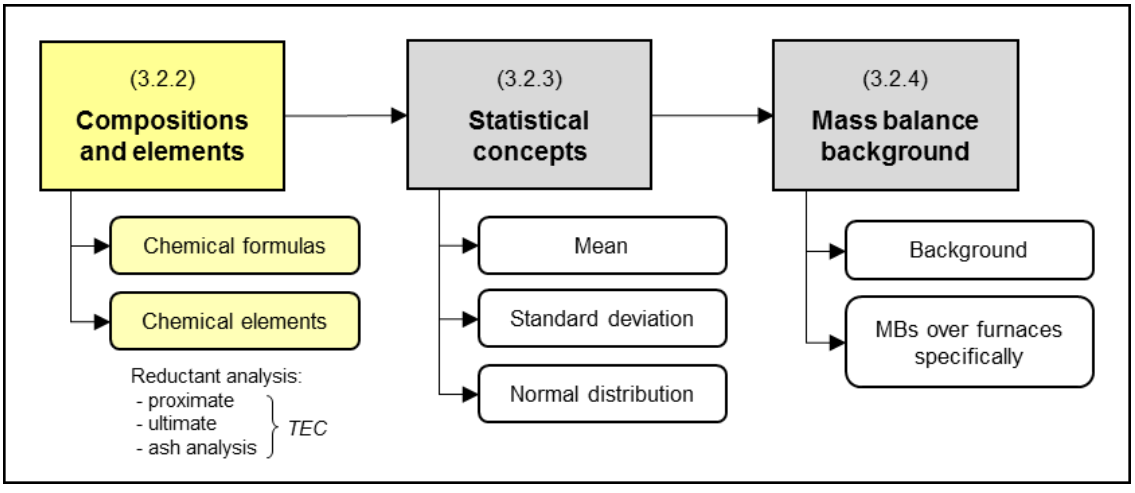


Figure 3-3: Illustration of literature study conduction (Section 3.2.2)

3.2.3 Statistical concepts

In order to perform an elemental mass balance over the furnace, the mass of each stream must be assigned to a corresponding composition. It is found that there are not necessarily compositional analyses done on a daily basis, even though the specific material is consumed by the furnace every day. Another constraint is the uncertainty of when or where the analyses were done. If the raw material samples were analysed upon arrival/delivery, the material could have been stored in silos or stockpiles for an undefined period, creating a buffer capacity between the time of analysis and the time of batching to the furnace.

Due to these constraints, it is not possible to match each day's batching mass with its corresponding composition. It is therefore necessary to use a representative average of the data to account for any data losses and buffer capacities. A brief research discussion on some relevant statistical concepts will therefore follow.

Mean value (μ)

The mean, or average, is the sum of the observed values in a dataset divided by the number of values in the dataset [139, 140]. The equation used to calculate the mean value of a dataset is given by Equation 3-14.

$$\mu = \frac{1}{n} \times \sum_{i=1}^{n} a_i$$

Equation 3-14: Mean (or average) value

Where:

n = Number of values in the dataset

$\sum_{i=1}^{n} a_i$ = Sum of all values in the dataset

Standard deviation (σ)

The standard deviation quantifies how concentrated the data is around the mean of the dataset. A large standard deviation implies that the data is less concentrated around the mean, and more spread out [141]. The equation used to calculate the standard deviation of a dataset is given by Equation 3-15.

$$\sigma = \sqrt{\frac{\sum(x - \bar{x})^2}{n}}$$

Equation 3-15: Standard deviation

Where:

n = Number of values in the dataset

x = Each value in the dataset

$\bar{x}$ = Average of the dataset

Normal distribution

If a large set of data is available for a certain measurement over a period of time, and it is required to use these values as one constant average value, there are certain things to keep in mind. A "normal distribution", also known as a "bell curve", is the distribution of data which occurs naturally in various situations [142, 143]. It is a frequency plot which is symmetrically distributed around the mean (μ) controlled by the standard deviation (σ) and resembling the shape of a bell. A normal distribution plot is shown in Figure 3-4 [144].

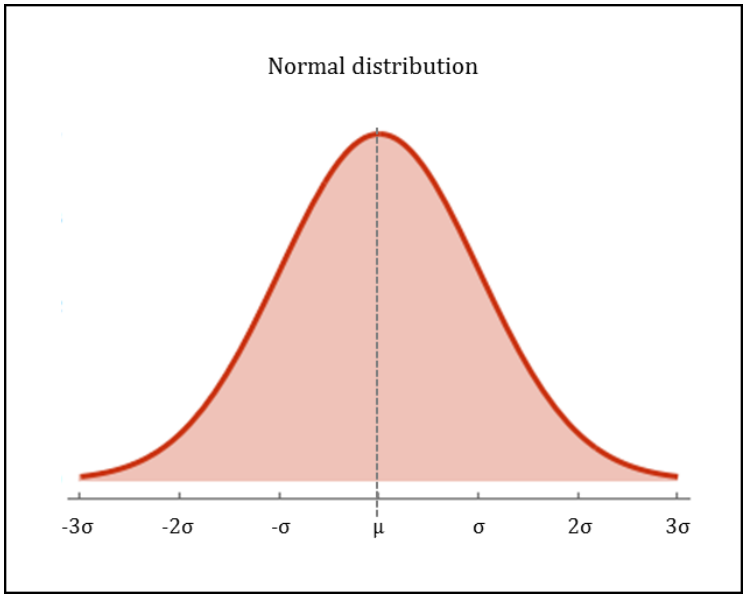


Figure 3-4: A typical normal distribution curve

The empirical rule (or the 68-95-99.7 rule) states the percentage of data which falls within a certain range for any normally distributed data [145]:

- 68% of the data will fall within one standard deviation (±σ) of the mean (μ)
- 95% of the data will fall within two standard deviations (±2σ) of the mean (μ)
- 99.7% of the data will fall within three standard deviations (±3σ) of the mean (μ)

If these rules apply to a dataset, the data is considered to be normally distributed. The three statements in this rule are illustrated in Figure 3-5.

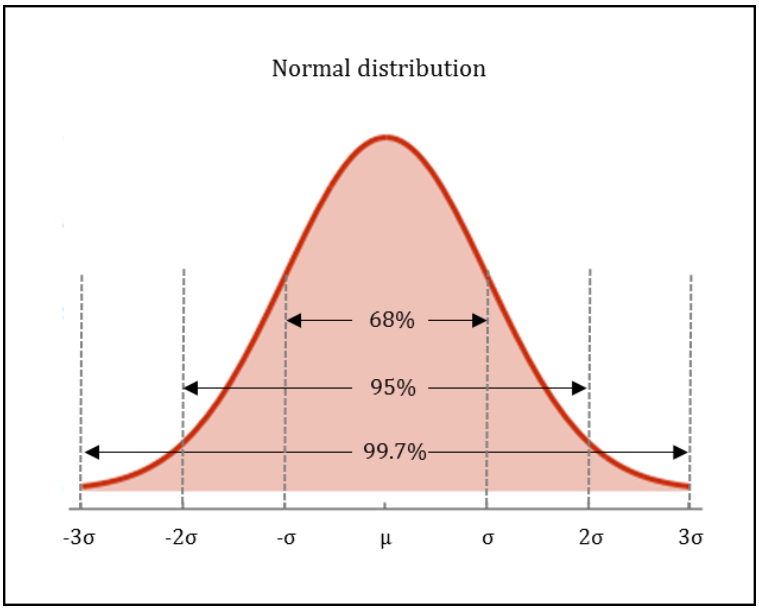


Figure 3-5: The empirical rule

If the data is considered to be normally distributed, it is highly likely that the mean, median and modus are all equal, and that the mean calculated from the dataset is representative [142].

This section provided information on relevant statistical concepts, which would aid in using a representative average of the data to account for any data losses and buffer capacities. The outline of this section is illustrated by the yellow highlighted blocks in Figure 3-6.

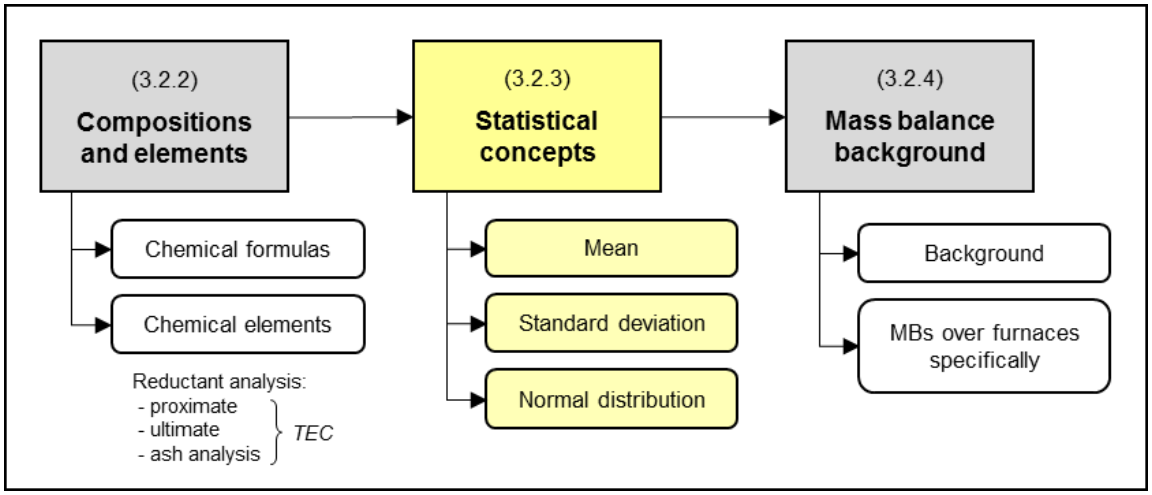


Figure 3-6: Illustration of literature study conduction (Section 3.2.3)

3.2.4 Mass balance research

The tier 3 calculation method is based on a basic mass balance approach. It is necessary to research the fundamentals of a mass balance method, and explore the application of mass balances on metal smelting furnace operations.

Background

A basic mass, or material balance, is based on the law of conservation of mass, which states that mass cannot be created or destroyed. A mass balance uses the principle of "mass in equals mass out" of a system in steady-state. Mass balances are generally used to solve the unknown mass flowrates and compositions of streams [146].

A material balance can be performed on the total mass entering and exiting the FeCr furnace, but is also based on the individual chemical elements. These two different approaches are shown in Figure 3-7, followed by Equation 3-16 and Equation 3-17, respectively:

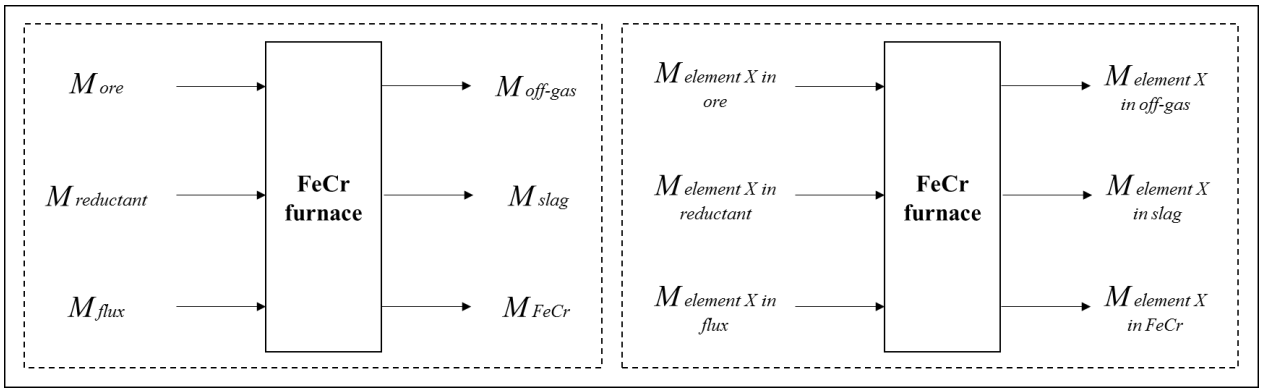


Figure 3-7: Illustrating a basic mass balance over a FeCr furnace

$$M_{ore} + M_{reductant} + M_{flux} = M_{FeCr} + M_{slag} + M_{off-gas}$$ *Equation 3-16: Overall mass balance*

$$\sum(M_{X_{in}}) = \sum(M_{X_{out}})$$ *Equation 3-17: Elemental mass balance*

Where *"M"* represents the total mass of a certain stream or element, and *"X"* refers to a certain chemical element.

Mass balances over a furnace

Even though literature for FeCr furnace mass balances is limited, a considerable amount of literature was found for mass balances over a blast furnace (steel-making).

Ruuska *et al.* [147] conducted a study on mass-balance-based multivariable modelling of a basic oxygen furnace (BOF). This was done to find practices for further improving the efficiency and controllability of the oxygen steelmaking. Various input and output streams are present at the BOF and the mass, and composition of these streams are essential to conducting a mass balance.

A study done by Bhattacharya & Muthusamy [148] focused on developing static heat-energy balance mathematical models for an iron-blast furnace. For one to prepare an accurate heat balance, a proper mass balance around the furnace is the first step. In order for this to be done, every material entering and exiting the furnace was evaluated, and the respective elemental compositions were calculated. All the major components and reactions of an iron blast furnace have been included in the study to accurately complete the mass, and ultimately heat balances.

Mandal *et al.* [149] evaluated a steady-state thermal and material balance model for an iron-making blast furnace and validated it with operational data. For the main reason to predict the off-gas composition and the raw material consumption, as well as an overall heat balance, a mathematical model has been developed over the blast furnace. The following relevant assumptions were made in the development of this input-output model (mass-balance):

- The process of iron making is done under steady state, i.e. mass in = mass out.
- The less prominent reactions, e.g. between N_2 and O_2 (to form NO), or N_2 and H_2 (to form NH_3), have been ignored.
- The composition of similar reductant was assumed to be equal.
- Oxides of aluminium (i.e. Al_2O_3) in the fluxes do not take part in any chemical reactions, and therefore remain unchanged in the slag phase.

The last assumption is confirmed by a study from the University of Technology of Iraq [150], stating that the total amount of CaO, MgO and Al_2O_3 will end up in the slag, unchanged.

According to Biermann *et al.* [26], a mass balance over a furnace would require a complete elemental analysis of all the input and output streams. The influence of raw material pre-treatments (such as pre-heating, drying, or pelletising) must also be considered. It is, once again, stated that all the CaO, MgO, and Al_2O_3 present in the feed (usually only through fluxes) can be assumed to report to the slag.

Another assumption that can be made is that the excess carbon and sulphur not forming part of the metal product will exit the furnace as part of the off-gas stream in the form of CO, CO_2 or SO_2. Moisture present amongst the raw materials will also exit as off-gas, along with all the N_2 within the system [26].

This section ultimately focussed on gathering information on mass balances, and the application of mass balances on metal-smelting furnace operations specifically. This is illustrated by the section layout (Section 3.2) in Figure 3-8.

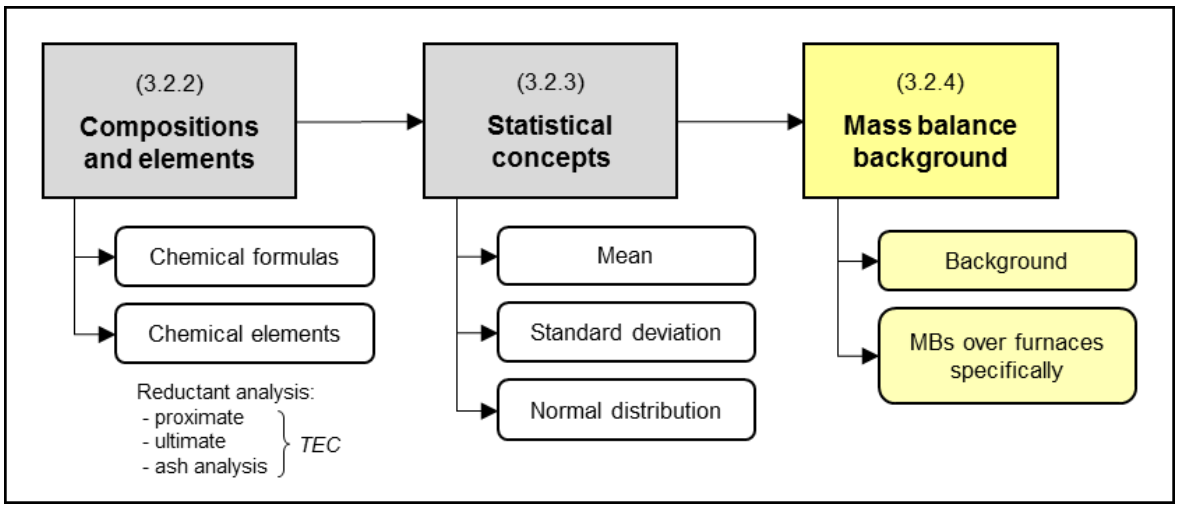


Figure 3-8: Illustration of literature study conduction (Section 3.2.4)

3.2.5 Research summary

The literature study provided information on relevant areas in order to gain knowledge for constructing a mass balance over a FeCr furnace. Based on the research done in Section 3.2, a list of assumptions is made (Table 3-2, below).

Table 3-2: List of assumptions

	Assumption:	Reference:
Streams and elements		
1	Ore, reductant, and fluxes enter a FeCr furnace, while FeCr product, slag, and off-gas exit the furnace; these streams consist of certain elements (see Table 3-1 for compositions).	[7, 14, 15]; [107 - 113]
2	Slag production is accurately calculated through a slag-to-metal ratio.	[130]
3	All mass and composition data from site is measured, transferred, stored, processed correctly.	[77]
FeCr process		
4	Monthly data resolution will encapsulate the total process of FeCr production (from raw materials batched until FeCr mass produced) [Assumed since some data is only obtained in monthly resolution.]	N/A
5	Composition of raw materials will remain constant from the sampling point until batching. [Assumed since raw materials may experience rainy or warm weather conditions after sampling, which may influence the analysis.]	N/A
6	For a normal distributed dataset, an annual constant composition is representative and will have no major effect on the results: - If compositions of feed materials are measured, an unknown buffer capacity (e.g. stockpiles) exist until batched - Sometimes compositions are not available consistently, i.e. a constant average must be used.	[142, 143, 144]
FeCr furnace and reactions		
7	FeCr production is a steady state process, i.e. mass in = mass out.	[149]
8	No material (carbon) from the furnace electrodes will react within and exit the system.	
9	No air is accounted for in MB calculations, since the amount of air in the system is unknown.	[149]
10	Oxides of aluminium (i.e. Al_2O_3) in the feed do not take part in any chemical reactions, and therefore remain unchanged in the slag phase.	[149, 150]
11	All carbon atoms present in the furnace off-gas will eventually be converted to CO_2.	[16]
12	Excess carbon and sulphur not forming part of the metal product will exit the furnace as part of the off-gas stream, in the form of CO, CO_2 or SO_2.	[26]
13	Moisture present amongst the raw materials will exit as off-gas, with all N_2 within the system.	[26]
Coal / ash analysis		
14	Fixed carbon + volatile matter + moisture + ash content = 100% of the coal sample weight.	[133]
15	Ultimate analysis + moisture + ash content = 100% total coal	[134, 135]
16	Ash analysis cannot be used for actual elements in raw ash (due to analysis process)	[138]
17	Bulletin coal data received is representative per each coal field, and coals from the same coal field will not vary significantly in composition.	[136]
18	The elements from the ash analysis will be regarded as “trace elements”, while the oxides from the ash analysis will not be considered as part of the original raw coal ash.	N/A
19	The TEC of different coal samples (Equation 3-8 to Equation 3-13) account for the major elements within the coal and is sufficient for the applications of this study.	N/A
20	All raw materials are wet when sampled for analyses, and when entering the furnace.	N/A

3.3 Methodology

3.3.1 Preamble

Section 1.3 noted that the prescribed CO_2 quantification methods are not necessarily accurate and that there is a need to refine these prescribed methods and investigate the potential for improvement. Section 3.2 reviewed the relevant literature needed do to a proper furnace system evaluation and conduct a detailed mass balance in order to estimate the CO_2 emissions from the furnace. The knowledge gained during this literature study was used for a generic approach to be developed on the construction of a detailed mass balance.

The approach developed (illustrated in Figure 3-9) includes seven main steps (purple block), whereas the first three steps correspond with the first three steps from the previous chapter (Section 2.3), indicated in the grey. The four newly added steps include assigning the compositions to its corresponding mass measurements, and constructing the mass balances (blue block), which is done in three different stages. This approach will be discussed in detail in Sections 3.3.2 to 3.3.7.

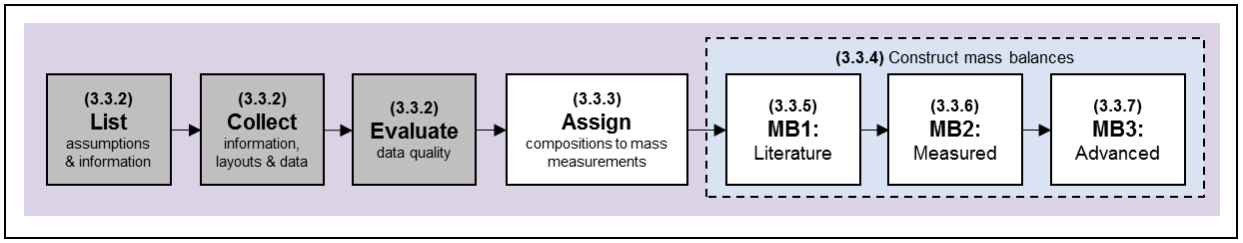


Figure 3-9: Approach to construct a detailed mass balance (MB) over a FeCr furnace

3.3.2 First three steps from Chapter 2

List of assumptions and information required

Listing the assumptions and requirements is an important step in preparing for all proceeding calculations to be done. In Chapter 2, a list of assumptions was constructed, based on knowledge gained from literature. This list is updated with relevant information obtained from Section 3.2, and is presented as Table 3-2 at the end of Section 3.2. The required information simply include all available mass and composition data (input and output streams), as discussed in Section 3.2.2.

Collection of information, layouts and data

The collection step involves obtaining layouts of the furnace, the relevant points of measurement indicated on layouts, as well as the corresponding mass and composition data for the evaluation period. See Section 2.3.3 for more detail regarding this step.

Data quality evaluation

When evaluating a FeCr furnace and preparing to conduct a mass balance, a significant amount of data needs to be collected, processed, and analysed. Thorough data evaluation is therefore necessary. To obtain more details regarding this step, see Section 2.2.5.

3.3.3 Assign compositions to mass data

After the relevant data is collected and evaluated, the next step is to assign the correct compositions to their corresponding mass parameters. These compositions refer to the total elemental composition (TEC) of all streams entering and exiting the furnace (ore, reductant flux, FeCr metal product, and slag). Note that this step is only applicable when data from site is available, otherwise literature values should be assumed. The assignment of compositions to mass measurements consists of three sub-steps, namely *Step 1: Estimate the total elemental composition of reductants*, *Step 2: Determine representative composition value*, *Step 3: Apply formula to calculate mass of all elements*. This step, with its three sub-steps, are illustrated in Figure 3-10.

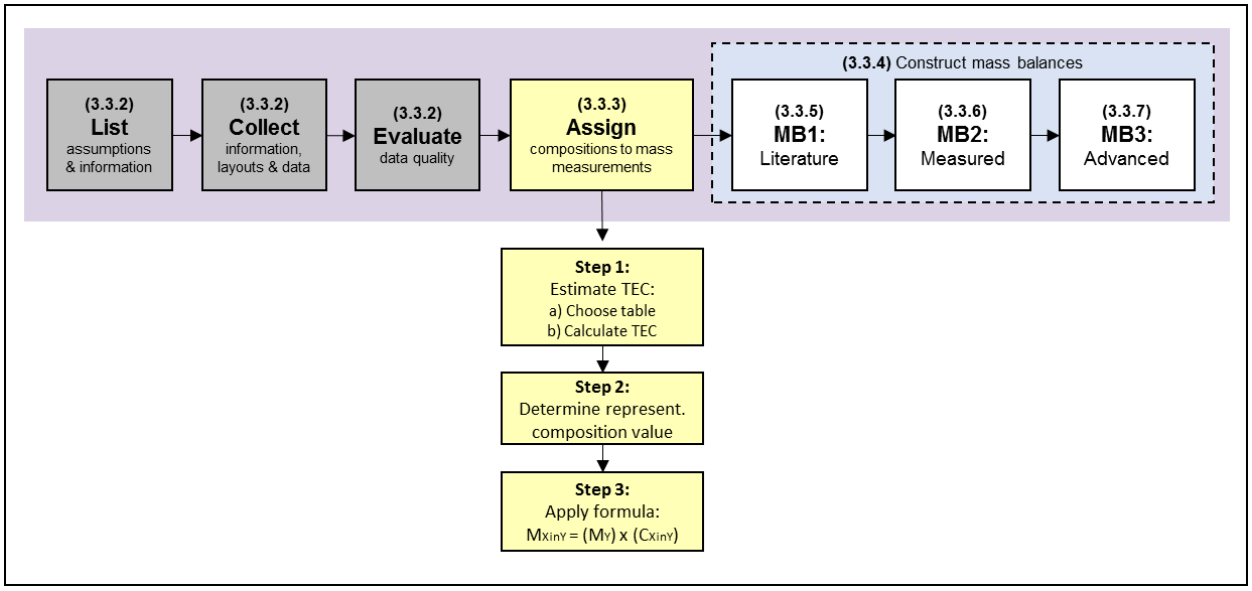


Figure 3-10: Approach to construct a detailed MB over a FeCr furnace (assignment step)

Step 1: Estimate the total elemental composition of reductants

From literature, compositions of the ore, flux, product and slag are often available, and give the mass percentage of each element present in the material. The reductant, however, can be analysed in various ways: proximate, ultimate and ash analysis (discussed in Section 3.2.2). From the calculations done in Section 3.2.2 and Appendix C, a simple two-step guide is constructed to aid in estimating the TEC of the specific reductants entering the furnace:

a) Choosing the relevant table to work from:

When reductant data is obtained from site, the description of the reductant is also usually given. Table 3-3 gives the relevant table to use, based on what information is known regarding the coal specifications.

Table 3-3: Indication of table to be used based on coal specifications known

Coal specifications known	Table to be used
Coal type and specific coal field is known	Table C-3
Coal type and province of origin is known	Table C-4
Only coal type is known	Table C-5

The outcome of this step is to choose one of the tables (Table C-3, Table C-4 or Table C-5), which can be located in Appendix C.

b) Use variables to calculate the TEC based on available data

Table 3-4 gives information on how to determine the TEC based on the information available.

Table 3-4: Indication on how to estimate the TEC of reductant

Reductant analysis data available from site or supplier	Variables to use to determine TEC of reductant
Proximate analysis	Use **ultimate** analysis data from the table chosen in *Step 1*, together with the specific **proximate** analysis data from site.
Ultimate analysis	Use **proximate** analysis data from the table chosen in *Step 1*, together with the specific **ultimate** analysis data from site.
Proximate -; ultimate analysis	Use the specific **proximate** and **ultimate** analysis data from site.

After this step, the variables to be used to estimate the TEC of the reductant material will be established, and can be plugged into Equation 3-8 to Equation 3-13 (Section 3.2.2) for the respective elements.

Step 2: Determine a representative composition value

The chemical compositions of all materials are known either from literature, or from site (data obtained). Figure 3-11 shows an example of composition data collected from site. It represents the data for a specific element (X) present in one of the material feed streams (Y) over a period of time, given in daily resolution.

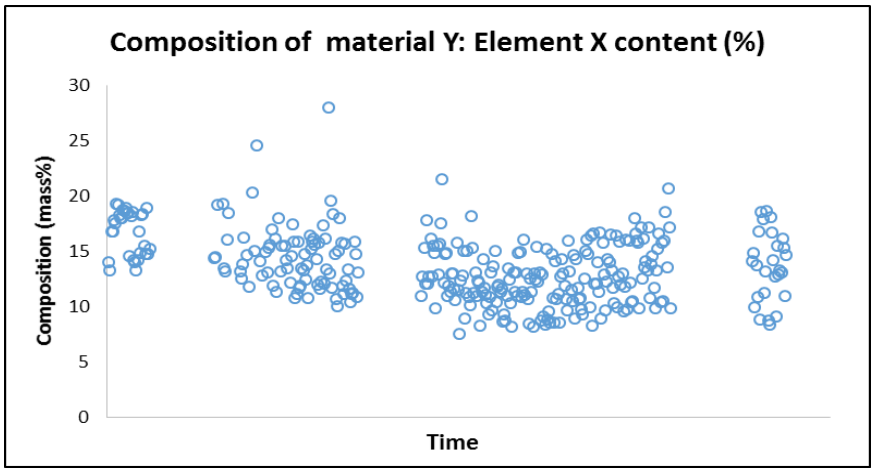


Figure 3-11: Composition data of material Y

It can be seen that there are some gaps in the data obtained and that there were no compositional analyses done every day necessarily, even though material Y was consumed every day. Another constraint in the credibility of this high-resolution data, is the fact that it is uncertain of when or where these analyses were done. If these raw material samples were analysed upon arrival/delivery, the material could have been stored in silos or stockpiles for an undefined period, creating a buffer capacity between the time of analysis and the time of batching to the furnace.

Due to these constraints, it is not possible to match each day's batching mass with its corresponding composition. It is therefore necessary to use a representative average of the data to account for any data losses and buffer capacities. Figure 3-12 illustrates an average (μ) of the dataset, calculated by Equation 3-14.

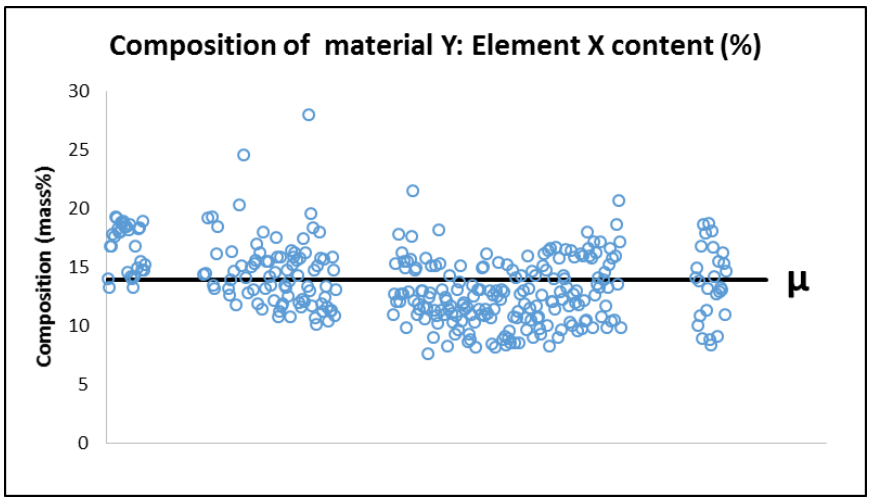


Figure 3-12: Composition data of material Y with average value

In order to determine whether this average value is representative of the dataset, it is necessary to evaluate the dataset. A standard deviation (σ) must be determined (see Equation 3-15) before a

two-standard deviation band width can be plotted onto the raw composition. This is shown in Figure 3-13.

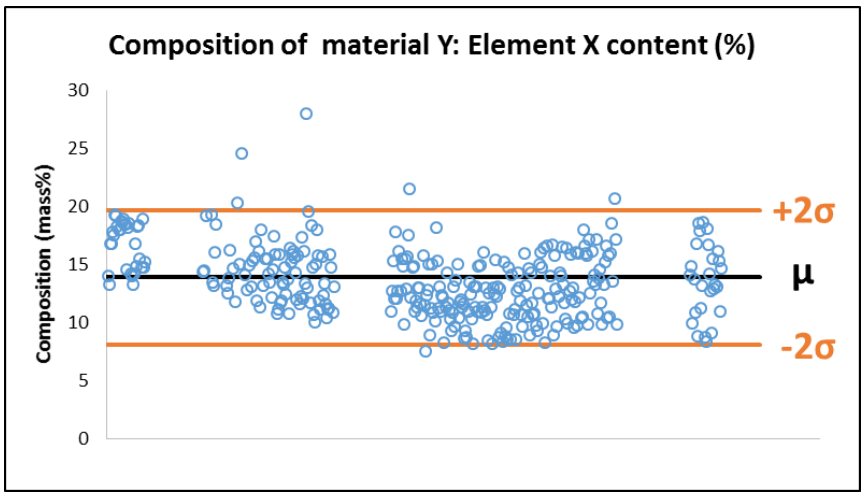


Figure 3-13: Composition data of material Y, average, and two standard deviations width

The dataset can then be tested for a "normal distribution", stating that more than 95% of the data will fall between -2σ and 2σ from the mean. If the dataset adheres to this rule, the data is assumed to be normally distributed and that the mean, median and modus are all equal. The average value (μ) calculated earlier is therefore assumed to be representative of the dataset and can be used as a constant average value.

Step 3: Determine mass of elements

Depending on the desired data resolution, the mass of each element in the furnace will be calculated by multiplying the composition (%) with the relevant mass, e.g.:

$$M_{X\ in\ Y} = M_Y \times C_{X\ in\ Y}$$ *Equation 3-18: Determining mass of element X in material Y*

Where,

$M_{X\ in\ Y}$ = Mass of element X present within material Y (to be calculated)

M_Y = Total mass of material Y

$C_{X\ in\ Y}$ = Composition percentage of element X present within material Y

After the mass of each element is calculated, the final step of the methodology presented in Figure 3-9 can be discussed.

3.3.4 Construct mass balances

The construction of the mass balances will take place over three stages: Mass balance based on literature (Section 3.3.5), mass balance based on measurements (Section 3.3.6), and the advanced mass balance (Section 3.3.7). Each one of these three mass balances will consist of six steps, namely *Step 1: Estimate slag mass, Step 2: Estimate off-gas mass, Step 3: Collect elemental compositions, Step 4: Determine mass of elements, Step 5: Estimate CO_2 emissions* and *Step 6: Calculate MB error*. This is illustrated in Figure 3-14.

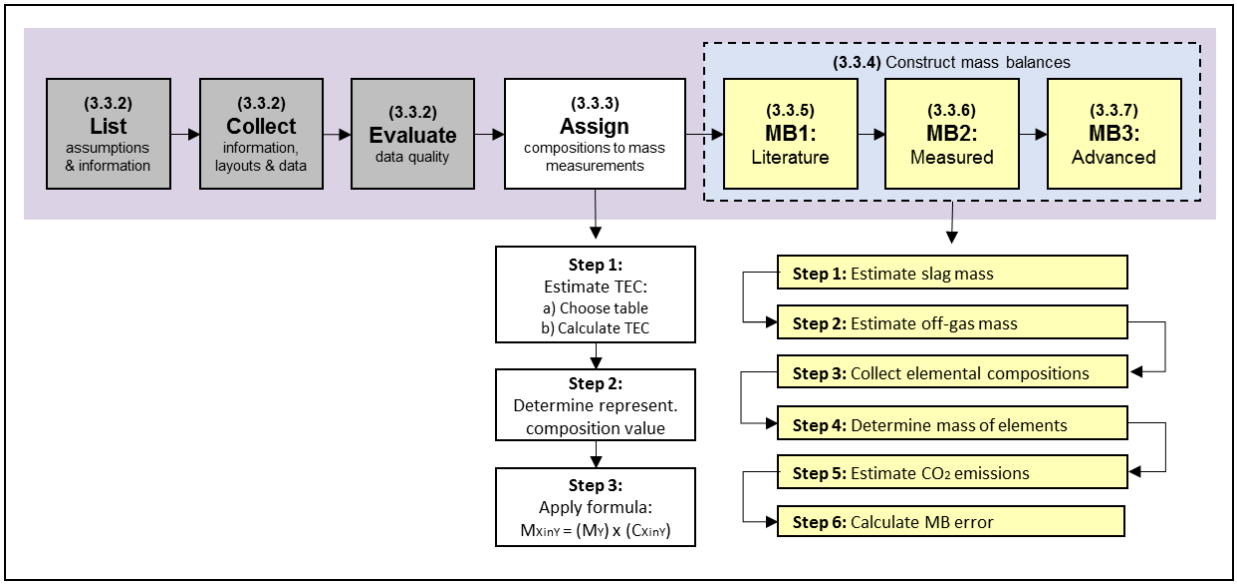


Figure 3-14: Approach to construct a detailed MB over a FeCr furnace (mass balance step)

Figure 3-15 shows a basic FeCr furnace layout with the relevant input and output streams.

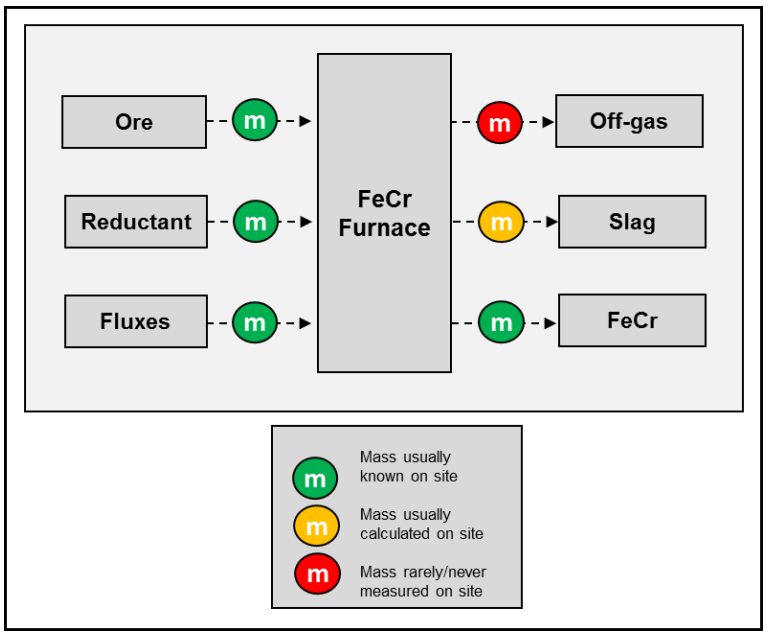


Figure 3-15: Basic FeCr furnace layout with input- and output stream POM

Figure 3-15 illustrates that the mass of the ore, reductant, fluxes and FeCr product are measured and known on site. The slag mass, however, is calculated by means of a slag-to-metal ratio, which is sampled irregularly, and not necessarily accurately. The off-gas mass is not measured. This layout will be used as basis for all mass balances to follow in the methodology section: Mass balance based on literature (Section 3.3.5), mass balance based on measurements (Section 3.3.6), and advanced mass balance (Section 3.3.7). Each one of the mass balances will be done by means of the six steps referred to in Figure 3-14.

3.3.5 Mass balance based on literature (MB1)

This first mass balance is based on assumptions of data/information from literature. Suppose the furnace is batched with 600 kg ore, 150 kg reductant (anthracite) and 100 kg fluxes (quartz), and it produces 280 kg FeCr metal product. Note that these measurements are not representative of a specific time period, and were chosen to simply illustrate the calculations that follow. The values used were randomly chosen to ease the illustration of the calculations. The mass values of the different streams are, however, within an operational/real-world ratio with one another.

Step 1: Estimate slag mass

An overall mass balance must be constructed in order to calculate the mass of the off-gas exiting the furnace. A constant slag-to-metal ratio is firstly assumed from literature (usually between 1.1 and 1.8 tonnes of slag produced per tonne of metal [130]) to calculate the slag mass. A slag-to-metal ratio of 1.45 is assumed (average of the values suggested by literature). Equation 3-19 illustrates the quantification of the slag mass through a slag-to-metal ratio.

$$M_{slag}\ (kg) = Slag\ to\ metal\ ratio\ \times M_{FeCr} \qquad \textit{Equation 3-19: Determining slag mass}$$

$$= 1.45\left(\frac{kg\ slag}{kg\ FeCr}\right) \times 280\ kg\ FeCr$$

$$= \mathbf{406\ kg}\ \text{slag produced}$$

Step 2: Estimate off-gas mass

Hereafter, an overall mass balance is done to estimate the off-gas mass by using Equation 3-16.

$$M_{ore} + M_{reductant} + M_{flux} = M_{FeCr} + M_{slag} + M_{off-gas}$$

$$M_{off-gas} = M_{ore} + M_{reductant} + M_{flux} - M_{FeCr} - M_{slag}$$

$$= 600\ kg + 150\ kg + 100\ kg - 280\ kg - 406\ kg$$

$$= \mathbf{164\ kg}\ \text{off-gas emitted}$$

Step 3 and 4: Collect elemental compositions and determine mass of elements

For the first mass balance, all compositions used will be **assumed from literature** (as from Table 3-1). Figure 3-16 shows how this table is used to calculate the mass of each element present in the furnace by applying Equation 3-18.

Material	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S
Cr ore	17.5	34.2	2.3	-	5.2	34.6	0.7	5.4	-	-	-
Anthracite	-	-	-	88.9	-	2.3	-	-	3.4	1.6	0.8
Char	-	-	-	77.8	-	21.1	-	-	0.3	0.7	-
Coke	-	-	-	89.0	-	-	-	-	3.6	1.6	5.0
Dolomite	-	-	-	13.0	-	52.0	22.0	13.0	-	-	-
Limestone	-	-	-	12.0	-	48.0	40.0	-	-	-	-
Quartz	-	-	47.0	-	-	53.0	-	-	-	-	-
Burnt lime	-	-	-	-	-	29.0	71.0	-	-	-	-
FeCr met	33.8	56.7	2.3	7.2	-	-	-	-	-	-	-
Slag	8.3	12.7	10.8	-	12.8	41.3	2.1	11.9	-	-	-
Off-gas	-	-	-	38.3	-	56.8	-	-	0.5	4.4	-

Cr ore	Comp. (%)	Calculation	Mass (kg)
Fe	17.5%	0.175 × 600 kg	105
Cr	34.2%	0.342 × 600 kg	205
Si	2.3%	0.023 × 600 kg	14
Al	5.2%	0.052 × 600 kg	31
O	34.6%	0.346 × 600 kg	208
Ca	0.7%	0.007 × 600 kg	4
Mg	5.4%	0.054 × 600 kg	32
Total	100%	-	600

Figure 3-16: Translating elemental compositions to elemental mass

Figure 3-16 highlights the translation of the elemental composition of the chrome ore specifically to the actual mass of each individual element present. The same process (Equation 3-18) is followed to estimate the elemental masses of all streams highlighted by this figure (anthracite, quartz, FeCr product, slag and off-gas). These results are given in Table 3-5.

Table 3-5: Elemental mass of input and output streams

Material	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Cr ore	105.0	205.3	14.0	-	31.2	207.9	4.3	32.4	-	-	-	0.0
Anthracite	-	0.0	0.0	133.4	-	3.5	-	-	5.1	2.3	1.2	4.5
Quartz	-	0.0	46.7	-	-	53.3	0.0	0.0	-	-	-	0.0
FeCr met	94.6	158.8	6.4	20.2	-	-	-	-	-	-	-	0.0
Slag	33.6	51.7	44.0	-	52.1	167.6	8.6	48.3	-	-	-	0.0
Off-gas	-	-	-	62.7	-	93.2	-	-	0.8	7.2	-	0.0

Step 5: Estimate CO_2 emissions

The amount of CO_2 emitted is assumed to be the amount of carbon in the off-gas stream x 44/12 (all C-atoms will eventually be converted to CO_2, according to assumption number 11 [Section 2.2: Table 3-2]). CO_2 emissions (kg) = 62.7 kg (yellow cell) × 44/12 = **230 kg CO_2**. Once the elemental mass of all streams is known, Equation 3-17 can be applied to perform a mass balance on every element present in the furnace in order to calculate the error of the first mass balance (*mass balance based on literature*). This is done to verify the **230 kg CO_2** result.

Step 6: Calculate MB error

Since all the input and output elements are already known (Table 3-5), Equation 3-17 will only be used as a check from which an error equation will be developed. Equation 3-17 states that $\Sigma X_{in} = \Sigma X_{out}$, meaning that the sum of all "X" elements entering the furnace must be equal to all the "X" elements exiting the furnace. If the element Cr is used as an example, the total Cr elements in must be equal to the total Cr elements out:

$$M_{Cr(in)} = Cr_{(ore)} + Cr_{(reductant)} + Cr_{(flux)} = 205.3\ kg + 0\ kg + 0\ kg = \mathbf{205.3\ kg}$$

$$M_{Cr(out)} = Cr_{(FeCr)} + Cr_{(slag)} + Cr_{(off-gas)} = 158.8\ kg + 51.7\ kg = \mathbf{210.5\ kg}$$

Since these two values are not equal to one another (205.3 kg ≠ 210.5 kg), it is evident that an error exists. This error can be estimated by the following equation:

$$Cr_{error} = \frac{M_{Cr(in)} - M_{Cr(out)}}{M_{Cr(in)}} \times 100\% = \frac{205.3 - 210.5}{205.3} \times 100\% = \mathbf{2.5\%}, \quad \text{or}$$

$$X_{error} = \frac{M_{X(in)} - M_{X(out)}}{M_{X(in)}} \times 100\%$$ *Equation 3-20: Elemental ("X") balance error*

After Equation 3-20 is applied to all elements, the following results are obtained (Table 3-6).

Table 3-6: Elemental balance error results

	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Total X_in	105.0	205.3	60.7	133.4	31.2	264.7	4.3	32.4	5.1	2.3	1.2	4.5
Total X_out	128.3	210.5	50.5	82.9	52.1	260.8	8.6	48.3	0.8	7.2	0.0	0.0
Error (%)	**22%**	**2.5%**	**17%**	**38%**	**67%**	**1%**	**102%**	**49%**	**84%**	**210%**	**100%**	**100%**

All elemental errors can now be used together to find a total error of the mass balance (*Literature mass balance*). A weighted factor will be used to normalise each elemental error and determine the total representative error. The weighted factor is calculated by dividing the elemental input mass (205.3 kg, for e.g. Cr) by the total input mass (850 kg). Equation 3-21 shows how this error is calculated, followed by an example for the Cr error.

$$Error\ (\%) = \sum \left(\frac{M_{X(in)}}{M_{Total(in)}} \times Elemental\ X_{error} \right)$$ *Equation 3-21: Total elemental balance error*

$$Error_{Cr}\ (\%) = \frac{205.3\ kg}{850\ kg} \times 2.5\% = \mathbf{0.6\%}$$

Equation 3-21 is applied to Table 3-6 and the results obtained are provided in Table 3-7. It is seen that the total *Literature mass balance* error is 17.5%.

Table 3-7: Total elemental balance error results (literature MB)

	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Total X_in	105.0	205.3	60.7	133.4	31.2	264.7	4.3	32.4	5.1	2.3	1.2	4.5
Total X_out	128.3	210.5	50.5	80.2	52.1	251.4	8.6	48.3	13.3	6.8	0.0	0.0
Error (%)	22%	3%	17%	38%	67%	1%	102%	49%	84%	210%	100%	100%
Total elemental balance error (%)	**2.7%**	**0.6%**	**1.2%**	**5.9%**	**2.5%**	**0.5%**	**0.5%**	**1.9%**	**0.5%**	**0.6%**	**0.1%**	**0.5%**

(2.7% + 0.6% + 1.2% + 5.9% + 2.5% + 0.5% + 0.5% + 1.9% + 0.5% + 0.6% + 0.1% + 0.5%)

= **17.5%**

i.e. CO_2 emissions = 230 kg ± 17.5% = **<u>230 kg ± 40 kg</u>**

Summary (MB1)

The *literature mass balance* is based on assumptions of data/information from literature. The slag mass was determined through a constant slag-to-metal ratio (from literature), after which the off-gas mass was determined. After this, the mass of each element entering and exiting the furnace could be calculated before the total elemental balance error was quantified. The CO_2 emissions were calculated to be 230 kg ± 40 kg. A mass balance error of 17.5% is significant, and does not suggest good balancing. The details regarding the six steps followed for the first mass balance are shown in Figure 3-17.

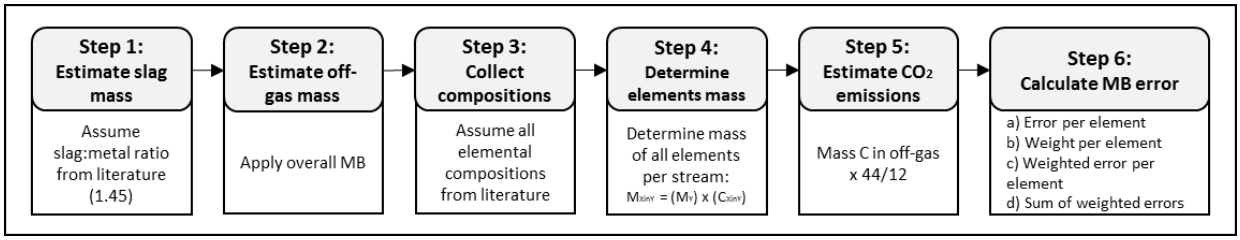


Figure 3-17: Six steps followed (Literature mass balance)

A next stage will be developed (*Mass balance based on measurements*) in order to obtain a better mass / elemental balance error over the furnace.

3.3.6 Mass balance based on measurements (MB2)

Where the first mass balance was based on assumptions of data/information from literature, the second is based on actual measurements from site. This means that for all the composition data assumed from literature in the previous mass balance (Table 3-1), these values will be substituted with actual, measured analysis composition values, where applicable. The same example will be used as with the previous mass balance, where the furnace is batched with 600 kg ore, 150 kg reductant (anthracite) and 100 kg fluxes (quartz), producing 280 kg FeCr metal product.

Step 1: Estimate slag mass

An overall mass balance must be constructed to calculate the mass of the off-gas exiting the furnace. Instead of assuming a constant slag-to-metal ratio from literature as with the first mass balance, the slag mass calculated by site personnel will be used, and assumed to be correct (even though slag mass is rarely measured, but rather calculated). Slag mass = 336 kg.

Step 2: Estimate off-gas mass

An overall mass balance can now be performed to estimate the off-gas mass (Equation 3-16).

$$M_{ore} + M_{reductant} + M_{flux} = M_{FeCr} + M_{slag} + M_{off-gas}$$

$$M_{off-gas} = M_{ore} + M_{reductant} + M_{flux} - M_{FeCr} - M_{slag}$$

$$= 600\ kg + 150\ kg + 100\ kg - 280\ kg - 336\ kg$$

$$= \mathbf{234\ kg}\ \text{off-gas emitted}$$

Step 3 and 4: Collect elemental compositions and determine mass of elements

The next steps allow for an elemental investigation where composition values will be taken from site-analysis data. Where no such data is available, literature values (from Table 3-1) will still be used. The data available is given in Table 3-8, where the only stream not analysed is the off-gas stream. The analysis values from literature will be assumed here, indicated in red text.

Table 3-8: Elemental composition analysis per stream

Material	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Cr ore	19.7	26.9	2.8	0.0	8.0	32.9	0.4	6.6	0.0	0.0	0.0	2.59
Anthracite	0.0	0.0	0.0	77.1	0.0	5.1	0.0	0.0	3.1	1.8	0.9	12.05
Quartz	0.2	0.0	46.0	0.0	0.5	53.0	0.1	0.1	0.0	0.0	0.0	0.09
FeCr met	37.9	48.6	4.4	6.7	0.0	0.0	0.0	0.0	0.0	0.0	0.1	2.30
Slag	3.5	6.2	13.7	0.0	15.1	42.8	3.9	12.7	0.0	0.0	0.2	1.86
Off-gas	-	-	-	**38.3**	-	**56.8**	-	-	**0.5**	**4.4**	-	-

Step 5 and 6: Estimate CO_2 emissions and calculate MB error

The steps followed and equations applied will be similar to that of the previous mass balance. After Equation 3-21 is applied in the final step, the elemental balance error results are obtained and provided in Table 3-9. It is seen that the total *measured mass balance* error is 10%.

Table 3-9: Total elemental balance error results (measured MB)

	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Total X_in	118.5	161.4	62.9	115.7	48.8	258.1	2.4	39.7	4.6	2.7	1.5	33.7
Total X_out	118.1	157.0	58.3	108.2	50.7	276.8	13.1	42.7	1.2	10.3	1.0	12.7
Error (%)	0%	3%	7%	6%	4%	7%	446%	8%	74%	283%	35%	62%
Total elemental balance error (%)	**0.1%**	**0.5%**	**0.5%**	**0.9%**	**0.2%**	**2.2%**	**1.3%**	**0.4%**	**0.4%**	**0.9%**	**0.1%**	**2.5%**

(0.1% + 0.5% + 0.5% + 0.9% + 0.2% + 2.2% + 1.3% + 0.4% + 0.4% + 0.9% + 0.1% + 2.5%)

= **10%**

i.e. CO_2 emissions = 328 kg ± 10.0% = **328 kg ± 33 kg**

Summary (MB2)

The *measured mass balance* is based on actual composition data, which is measured on site or by the supplier. The slag mass was assumed to be correctly "measured"/determined on site, after which the off-gas mass was determined. After this, the mass of each element entering and exiting the furnace could be calculated before the total elemental balance error could be quantified. The CO_2 emissions were calculated to be 328 kg ± 33 kg. The error value was determined as 10%, which shows a significant improvement from the previous MB (error = 17.5%). The details regarding the six steps followed for the second mass balance are shown in Figure 3-18.

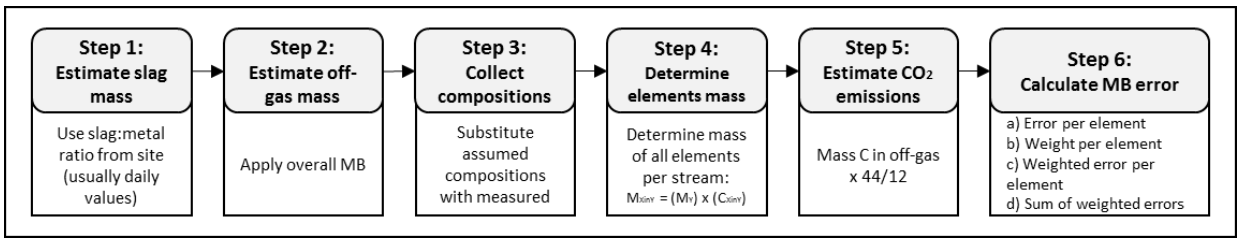


Figure 3-18: Six steps followed (Measured mass balance)

A final phase will be developed (*Advanced mass balance*) in order to obtain an even better mass / elemental balance error over the furnace.

3.3.7 Advanced mass balance (MB3)

Where the first and second mass balances were based on assumptions of data/information from literature, or actual measurements from site, the final mass balance will require more intuitive thinking, which will be based on FeCr knowledge obtained throughout this study. Once again, the furnace is batched with 600 kg ore, 150 kg reductant (anthracite) and 100 kg fluxes (quartz), and that it produces 280 kg FeCr metal product.

Step 1: Estimate slag mass

Firstly, a slag mass must be determined before the overall mass balance can be constructed to calculate the mass of the off-gas exiting the furnace. Instead of using the slag mass calculated by site personnel, the mass of the slag will be calculated in a different manner:

As with assumption number 10 (from the list of assumptions at the end of Section 2.2: Table 3-2), it is stated that oxides of aluminium (Al_2O_3) in the feed do not take part in any chemical reactions, and therefore remain unchanged in the slag phase. Since the composition of all Al_2O_3-containing feed streams are known, the amount of Al_2O_3 entering the furnace can be calculated. The ore stream contains 15.19% Al_2O_3, whereas the quartz contain only 0.98%. Therefore, the total amount of Al_2O_3 entering the furnace is:

$$M_{Al2O3(in)} = M_{Al2O3_{ore}} + M_{Al2O3_{quartz}}$$

$$= (600\ kg\ ore \times 15.19\%\ Al_2O_3) + (100\ kg\ quartz \times 0.98\%\ Al_2O_3)$$

$$= (91.14\ kg\ Al_2O_3) + (0.98\ kg\ Al_2O_3)$$

$$= \mathbf{92.12\ kg\ Al_2O_3}$$

It is assumed that the total amount of Al_2O_3 entering the furnace will exit the furnace in the slag phase. The slag composition is also measured, containing 28.53% Al_2O_3. The slag mass can thus be calculated by dividing the total Al_2O_3 entering the furnace by the Al_2O_3 composition of the slag stream (equation):

$$M_{slag} = \frac{M_{Al2O3(in)}}{C_{Al2O3_{slag}}}$$

Equation 3-22: Slag mass estimation from Al_2O_3

$$M_{slag} = \frac{92.12\ kg\ Al_2O_3}{28.53\%} = \mathbf{322.9\ kg\ slag}$$

Step 2: Estimate off-gas mass

The overall mass balance can now be performed to estimate the off-gas mass (Equation 3-16).

$$M_{ore} + M_{reductant} + M_{flux} = M_{FeCr} + M_{slag} + M_{off-gas}$$

$$M_{off-gas} = M_{ore} + M_{reductant} + M_{flux} - M_{FeCr} - M_{slag}$$

$$= 600\ kg + 150\ kg + 100\ kg - 280\ kg - 322.9\ kg$$

$$= \mathbf{247\ kg}\ \text{off-gas emitted}$$

Step 3 and 4: Collect elemental compositions and determine mass of elements

Since the off-gas is the only unmeasured stream (composition), this step allows for an elemental balance to quantify the off-gas composition. Equation 3-17 will be applied for all elements present in the off-gas (C, H, O, N, S) to determine its composition. Only carbon will be showcased:

$$\sum(M_{C_{in}}) = \sum(M_{C_{out}})$$

$$M_{C_{off-gas}} = \overset{=0}{M_{C_{ore}}} + M_{C_{reductant}} + \overset{=0}{M_{C_{flux}}} - M_{C_{FeCr}} - \overset{=0}{M_{C_{slag}}}$$

$$M_{C_{off-gas}} = (0) + (150\ kg \times 77.1\%) + (0) - (280\ kg \times 6.7\%) - (0)$$

$$M_{C_{off-gas}} = \mathbf{97\ kg\ C\ in\ off\text{-}gas}$$

The carbon composition of the off-gas is calculated by dividing the amount of carbon in the off-gas stream by the total amount of off-gas:

$$C_{C_{off-gas}} = \left(\frac{M_{C_{off-gas}}}{M_{off-gas}}\right) \times 100\% = \left(\frac{97\ kg\ C}{247\ kg\ off-gas}\right) \times 100\% = \mathbf{39\%\ C\ in\ off\text{-}gas}$$

The calculations are repeated for H, O, N, S, and the following results are obtained (Table 3-10):

Table 3-10: Off-gas composition analysis

Stream	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Off-gas	-	-	-	**39.2**	-	**48.5**	-	-	**1.9**	**1.1**	**0.2**	-

Step 5 and 6: Estimate CO_2 emissions and calculate MB error

The rest of the steps followed and equations applied will be similar to that of the previous mass balances. After Equation 3-21 is applied in the final step, the elemental balance error results are obtained and provided in Table 3-11. It is seen that the total *advanced mass balance* error is 2.8%.

Table 3-11: Total elemental balance error results (advanced MB)

	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Total X_in	118.5	161.4	62.9	115.7	48.8	258.1	2.4	39.7	4.6	2.7	1.5	33.7
Total X_out	117.6	156.1	56.5	115.7	48.8	258.1	12.6	41.1	4.6	2.7	1.5	33.7
Error (%)	1%	3%	10%	0%	0%	0%	425%	3%	0%	0%	0%	0%
Total elemental balance error (%)	**0.1%**	**0.6%**	**0.7%**	**0.0%**	**0.0%**	**0.0%**	**1.2%**	**0.2%**	**0.0%**	**0.0%**	**0.0%**	**0.0%**

(0.1% + 0.6% + 0.7% + 0.0% + 0.0% + 0.0% + 1.2% + 0.2% + 0.0% + 0.0% + 0.0% + 0.0%)

= **2.8%**

i.e. CO_2 emissions = 356 kg ± 2.8% = **356 kg ± 10 kg**

Summary (MB3)

The *advanced mass balance* calculated the slag mass by investigating the amount of Al_2O_3 in the feed and in the slag, after which the off-gas mass was determined. After this, the composition of the off-gas was determined and compared to literature. All elements entering and exiting the furnace were calculated before the total elemental balance error could be quantified. This error value was determined as **2.8%**, which shows a significant decrease from the previous MB (10%). The details regarding the six steps followed for the third mass balance are shown in Figure 3-19.

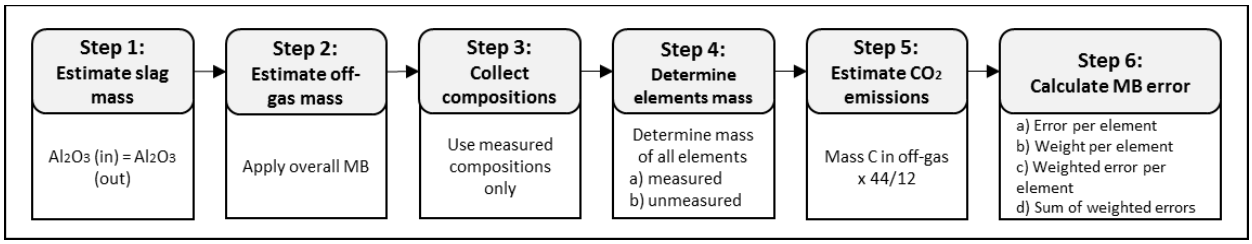


Figure 3-19: Six steps followed (Advanced mass balance)

All three mass balance stages use methods, assumptions or calculations gained from literature. It is evident that, for this example furnace, the *measured mass balance* (error = 10.0%) gives more accurate results than the *literature mass balance* (error = 17.5%), while the *advanced mass balance* (error = 2.8%) give more accurate results than the *measured mass balance* (error = 10.0%). The CO_2 emissions were calculated to be 356 kg ± 10 kg.

This methodology will be simplified in the next section: "Methodology summary".

3.3.8 Methodology summary

An approach was developed to construct various mass balances around the FeCr in order to estimate the CO_2 emissions in a more complex, yet more accurate manner. The three mass balance approaches evaluated included the *literature* mass balance, the *measured* mass balance and the *advanced* mass balance. The full strategy developed in Section 3.3 is based on the research done in Section 3.2, and is summarised in Figure 3-20. The details regarding the mass balance construction steps (blue block) are given in Table 3-12 on the next page.

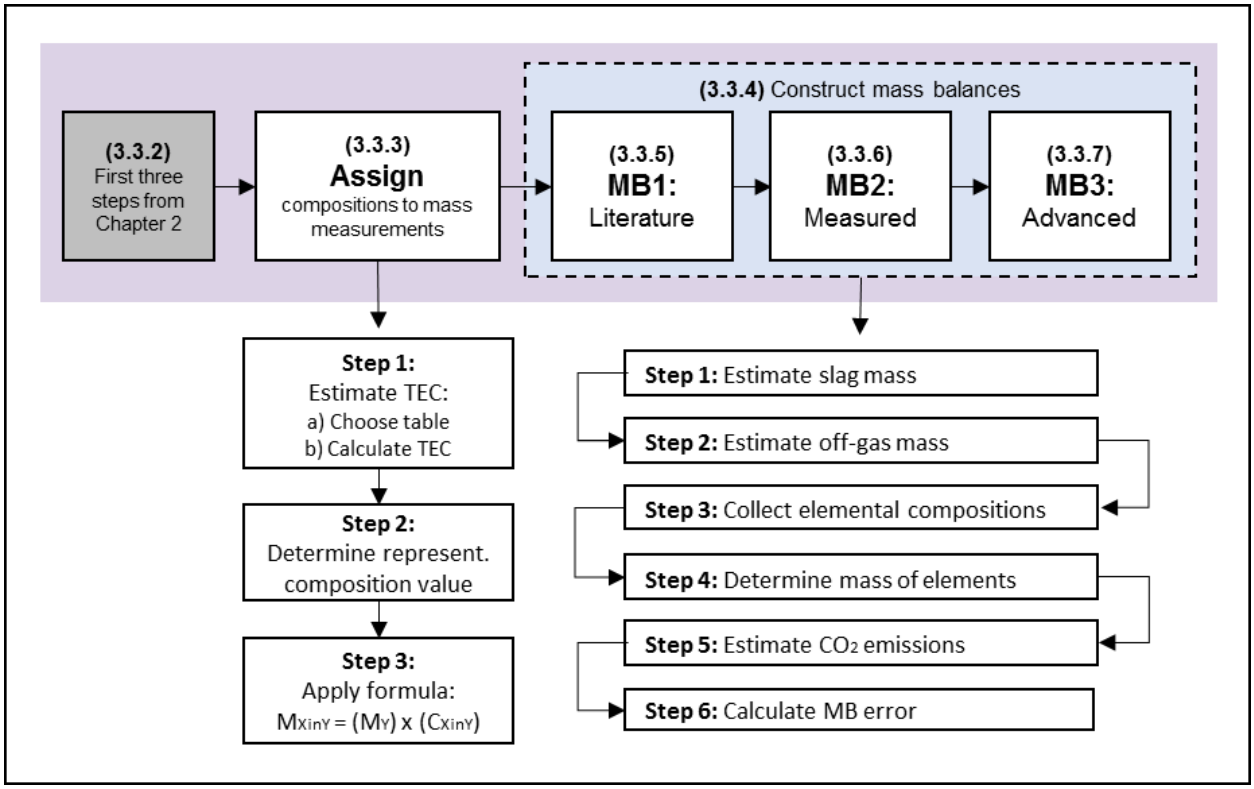


Figure 3-20: Summary of mass balance methodology

Table 3-12: Summary of steps for constructing the three mass balances

Steps to be followed	*MB1:* **Literature**	*MB2:* **Measurement**	*MB3:* **Advanced**
Step 1: **Estimate slag mass**	Assume slag:metal ratio from literature (1.45)	Use slag:metal ratio from site (usually daily values)	Al_2O_3 (in) = Al_2O_3 (out)
Step 2: **Estimate off-gas mass**	Apply overall MB	Apply overall MB	Apply overall MB
Step 3: **Collect compositions**	Assume all elemental compositions from literature	Substitute assumed compositions with measured	Use measured compositions only
Step 4: **Determine elements mass**	Determine mass of all elements per stream: $M_{XinY} = (M_Y) \times (C_{XinY})$	Determine mass of all elements per stream: $M_{XinY} = (M_Y) \times (C_{XinY})$	Determine mass of all elements a) measured b) unmeasured
Step 5: **Estimate CO_2 emissions**	Mass carbon (C) in off-gas × 44/12	Mass carbon (C) in off-gas × 44/12	Mass carbon (C) in off-gas × 44/12
Step 6: **Calculate MB error**	a) Error per element b) Weight per element c) Weighted error per element d) Sum of weighted errors	a) Error per element b) Weight per element c) Weighted error per element d) Sum of weighted errors	a) Error per element b) Weight per element c) Weighted error per element d) Sum of weighted errors

In the next section, this approach will be used and applied to real-life FeCr furnaces (case studies). These case studies will illustrate each of the three mass balance stages (*literature mass balance*, *measured mass balance*, and *advanced mass balance*).

3.4 Case studies: Results and discussion

3.4.1 Preamble

The previous section presented a method to follow for constructing a mass balance over a FeCr furnace. This mass balance is done to calculate the CO_2 emissions from the furnace as accurately as possible. Three detailed case studies (CS) will be used to showcase each one of the three mass balance stages: CS1) *literature* mass balance (Section 3.4.3), CS2) *measured* mass balance (Section 3.4.4), and CS3) *advanced* mass balance (Section 3.4.5).

3.4.2 Case study background

Information, the relevant points of measure and the corresponding mass and composition data over a three-year evaluation period have been collected for Furnace X. Note that this is the same furnace used in the case studies for Chapter 2 (Section 2.4). This is shown in Figure 3-21 (Figure 2-11).

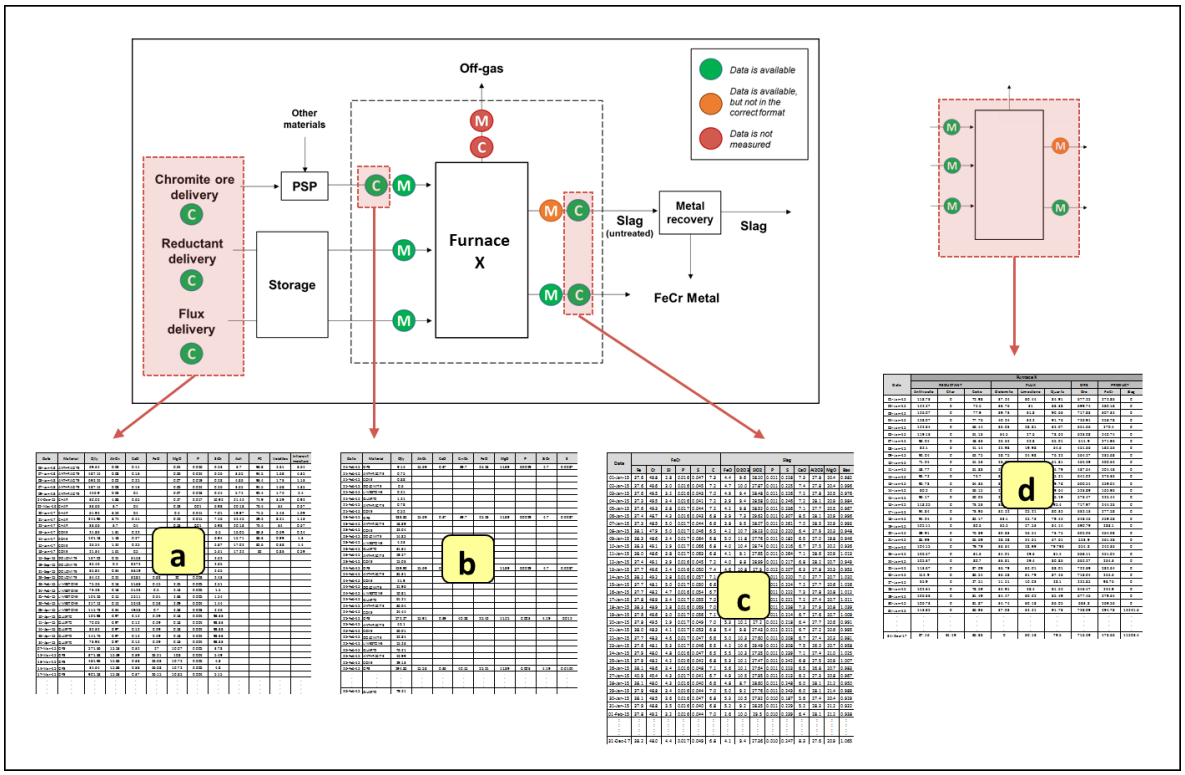


Figure 3-21: Collect information, layouts, and data (repeat of Figure 2-11)

Chrome ore, reductant (anthracite, char, and coke), and fluxes (dolomite, limestone, and quartz) are sampled on delivery (dataset “a”). Chromite ore is pelletised (PSP), and sampled again before batching (dataset “b”). The composition of the FeCr metal and slag is also determined when exiting the furnace (dataset “c”). The mass of all raw materials is determined in weigh bins right before

batching, whereas the FeCr metal and slag mass are measured at weighbridges (dataset "d"). Note that the slag mass meter is indicated in orange. This is due to the slag mass being determined by calculation, and not a physical mass-metering device. The slag mass is logged per month, but the rest of the data is in daily resolution. Thus, all data is converted to monthly resolution. This information is summarised in Table 3-13.

Table 3-13: Summary of available data (1)

Data-set	Type of measurement	Material	Unit	Data resolution	More information
"a"	Composition analysis	Chrome ore	%	Daily	Raw ore, before PSP
		Reductant (anthracite, char, coke)	%	Daily	Proximate analysis
		Fluxes (dolomite, limestone, quartz)	%	Daily	
"b"	Composition analysis	Chrome ore	%	Daily	After PSP
"c"	Composition analysis	FeCr metal	%	Daily	
		Slag	%	Daily	
"d"	Mass measurement	Chrome ore	Tonnes	Daily	Weigh bins
		Reductant (anthracite, char, coke)	Tonnes	Daily	Weigh bins
		Fluxes (dolomite, limestone, quartz)	Tonnes	Daily	Weigh bins
		FeCr metal	Tonnes	Daily	Weighbridges
		Slag	Tonnes	Monthly	Calculation

**All percentages (%) are based on mass percentages (%)*

The data available of what is actually required is shown in Table 3-14. The slag mass is calculated, while neither the off-gas mass nor composition is measured. All other parameters are measured.

Table 3-14: Summary of available data (2)

Stream	Type of composition	Available/measured?
Chrome ore	Mass	✓
	Composition	✓
Reductant	Mass	✓
	Composition	✓
Fluxes	Mass	✓
	Composition	✓
FeCr metal	Mass	✓
	Composition	✓
Slag	Mass	?
	Composition	✓
Off-gas	Mass	×
	Composition	×

Due to the first three steps of the methodology (developed in Section 3.3) originating from Chapter 2, these will not be discussed again. Also, the "Assign composition to mass data" step was illustrated in the literature study (3.2.2 and 3.2.3) and in the methodology section (3.3.3). The case studies will therefore only highlight the construction of mass balances, which is the core focus of this chapter.

3.4.3 Case study 1: Mass balance based on literature

This case study uses a mass balance based on assumptions of data/information from literature. For *step 1 and 2*, an overall mass balance must be constructed in order to calculate the mass of the off-gas exiting the furnace, since this is not measured. After a constant slag-to-metal ratio of 1.45 is assumed from literature [130], Equation 3-19 can be used to quantify the slag mass through this ratio. The equation is applied to data over a 36-month period. After the slag mass is known, the overall mass balance can be done to estimate the off-gas mass by using Equation 3-16. The results are shown in the overall mass balance graph (Figure 3-22).

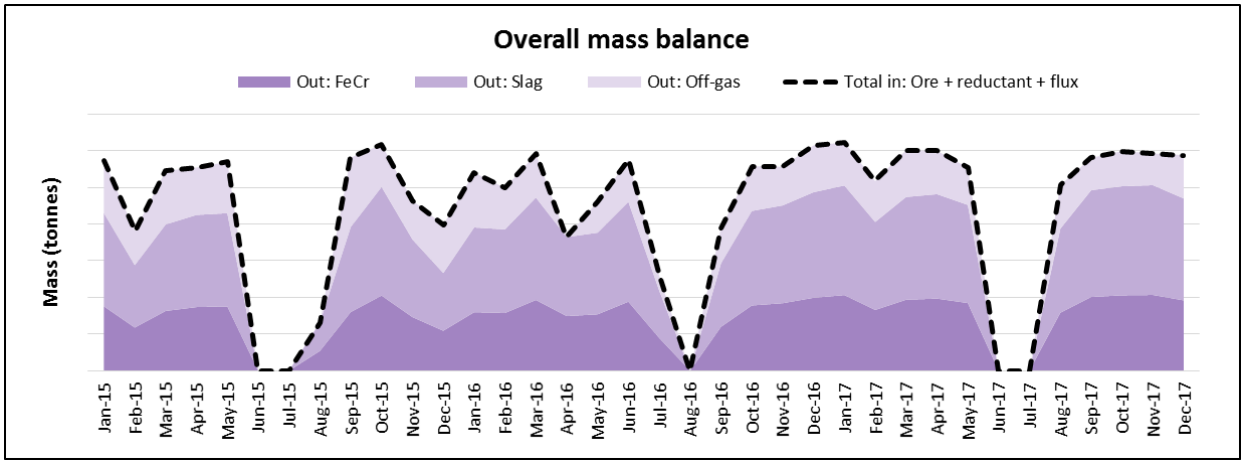


Figure 3-22: Overall mass balance trend (CS1)

Figure 3-22 illustrates that the sum of the three "out" streams (FeCr, slag and off-gas) are equal to the sum of the three "in" streams (ore, reductant and fluxes) throughout the whole 36-month period. Now that the off-gas mass is known, one can proceed to *step 3 and 4*.

Steps 3 and 4 allow for an elemental balance where all compositions used will be assumed from literature (as from Table 3-1). By applying Equation 3-18, the translation of the elemental composition to the actual mass of each individual element present can be accomplished. This is done over a period of 36 months, and the results of some prominent elements (Fe, Cr and C) are provided in Figure 3-23.

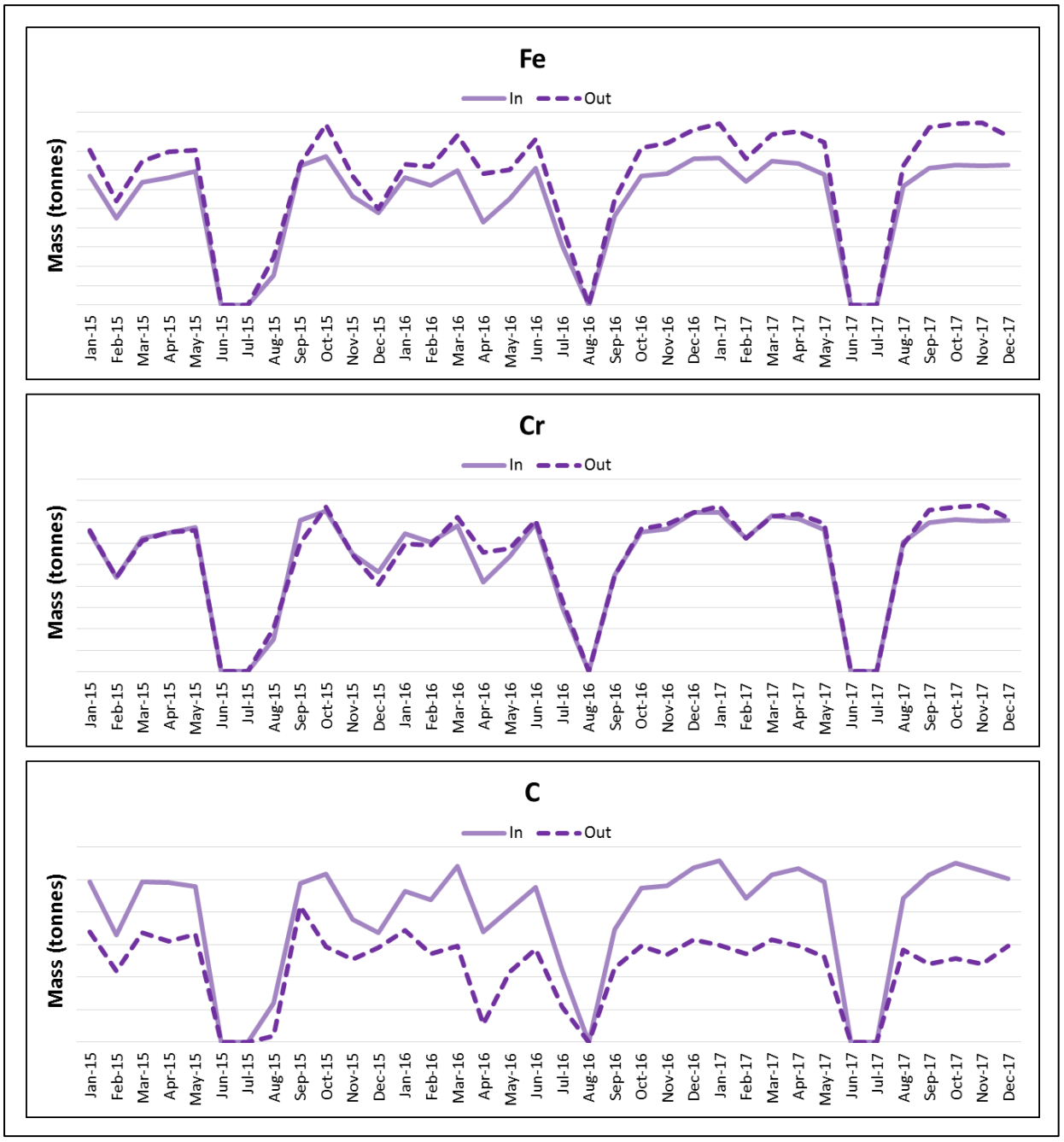


Figure 3-23: Elemental (Fe, Cr, C) mass balance trends (CS1)

It is clear that the amount of elements entering the furnace is not necessarily equal to that exiting. An error thus exists for each individual element, and will be determined later on.

After each element entering and exiting the furnace was calculated, the total amount of CO_2 emissions (tonnes) for each year respectively is determined (*step 5*):

Year 1 (Jan – Dec 2015): 22 805 tonnes × 44/12 = 83 620 tonnes CO_2

Year 2 (Jan – Dec 2016): 20 491 tonnes × 44/12 = 75 134 tonnes CO_2

Year 3 (Jan – Dec 2017): 20 743 tonnes × 44/12 = 76 057 tonnes CO_2

Even though three years' data is available, only the last year (2017) will be evaluated. Chapter 4 will eventually compare the results of 17 different furnaces, which will be done for one year's data.

Once the elemental mass of all streams are known, Equation 3-17 can be derived to perform a mass balance on every element present in the furnace in order to calculate the error of the mass balance (*step 6*). This is done to verify the total CO_2 emissions calculated for 2017 (76 057 tonnes). Equation 3-20 and Equation 3-21 are applied, and the results are shown in Table 3-15.

Table 3-15: Total elemental balance error results (CS1)

	Fe	**Cr**	**Si**	**C**	**Al**	**O**	**Ca**	**Mg**	**H**	**N**	**S**	**Trace**
Total X_in	35 330	69 067	14 506	50 833	10 498	87 474	4 619	10 902	1 710	812	1 313	966
Total X_out	43 717	71 728	17 202	27 614	17 766	87 932	2 945	16 464	278	2 386	0	0
Error (%)	24%	4%	19%	46%	69%	1%	36%	51%	84%	194%	100%	100%
Total elemental balance error (%)	**2.9%**	**0.9%**	**0.9%**	**8.1%**	**2.5%**	**0.2%**	**0.6%**	**1.9%**	**0.5%**	**0.5%**	**0.5%**	**0.3%**

The total mass balance error is calculated at 19.9% (sum of all "total elemental balance errors"). This means that the total CO_2 emissions = 76 057 tonnes ± 19.9% = 76 057 tonnes ± 15 106 tonnes.

CS1 summary

This case study was based on assumptions from literature. The slag mass was determined through a constant ratio from literature, after which the off-gas mass was determined. After this, the mass of each element entering and exiting the furnace could be calculated, before the total elemental balance error (19.9%) was quantified. The CO_2 emissions were calculated to be 76 057 tonnes ± 15 106 tonnes. More details regarding this case study can be found in Appendix F.

3.4.4 Case study 2: Mass balance based on measurements

This case study focuses on a mass balance, which is based on actual measurements from site (instead of on literature values as in CS1). This means that for all the composition data assumed from literature in the previous mass balance (Table 3-1), these values will be substituted with actual, measured analysis composition values from site, where applicable.

For *step 1 and 2*, an overall mass balance is performed to calculate the off-gas mass. Slag mass data from site is available and will be used for this balance. This is assumed to be correct, even though slag mass is rarely measured, but rather calculated. Since the ore, reductant, flux, FeCr product and slag streams' mass are now known, Equation 3-16 can be applied to estimate the

off-gas mass. The results are shown in the overall mass balance trend (Figure 3-24).

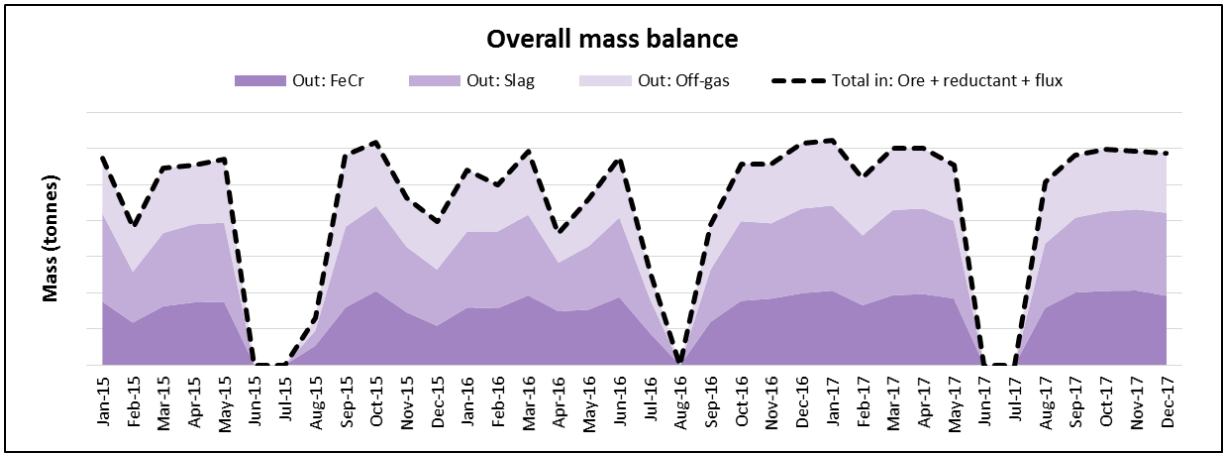


Figure 3-24: Overall mass balance trend (CS2)

Now that the mass of all streams (ore, reductant, flux, FeCr, slag and off-gas) are known, *steps 3 and 4* can commence. These steps focus on the elemental investigation where composition values from site analysis data will be used. If such data is not available, literature values will still be used. The off-gas is the only stream which composition is not measured (refer to Table 3-14), whereas the reductant analysis is done by proximate analysis only (refer to Table 3-13).

Table 3-3 and Table 3-4 (Section 3.3.3) can be used to provide guidance on determining the TEC of the reductants from the proximate analysis. The relevant variables were used, plugged into Equation 3-8 to Equation 3-13 (Section 3.2.2), and the TEC of each reductant type was estimated. Details on these calculations can be found in Appendix F.

The composition data is provided in Table 3-16 (as percentages, %), where the off-gas values are assumed from literature (Table 3-1), and the reductant values calculated based on Section 3.3.3.

Table 3-16: Elemental composition analysis per stream (CS2)

Material	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Ore	19.7	26.9	2.8	0.0	8.0	32.9	0.4	6.6	0.0	0.0	0.0	2.6
Anthracite	0.0	0.0	0.0	73.4	0.0	5.0	0.0	0.0	2.9	1.7	0.9	16.1
Char	0.0	0.0	0.0	61.6	0.0	13.1	0.0	0.0	4.3	1.4	0.7	18.9
Coke	0.0	0.0	0.0	74.4	0.0	6.8	0.0	0.0	3.2	1.7	0.9	12.9
Dolomite	0.5	0.0	1.2	5.9	0.2	42.2	31.5	18.5	0.0	0.0	0.0	0.0
Limestone	0.5	0.0	0.8	5.3	0.3	38.1	52.4	2.5	0.0	0.0	0.0	0.0
Quartz	0.2	0.0	46.0	0.0	0.5	53.0	0.1	0.1	0.0	0.0	0.0	0.1
Metal	37.9	48.6	4.4	6.7	0.0	0.0	0.0	0.0	0.0	0.0	0.1	2.3
Slag	3.5	6.2	13.7	0.0	15.1	42.8	3.9	12.7	0.0	0.0	0.2	1.8

By applying Equation 3-18, the translation of the elemental composition to the actual mass of each individual element present can be accomplished. The results of some prominent elements (Fe, Cr and C) are provided in Figure 3-25.

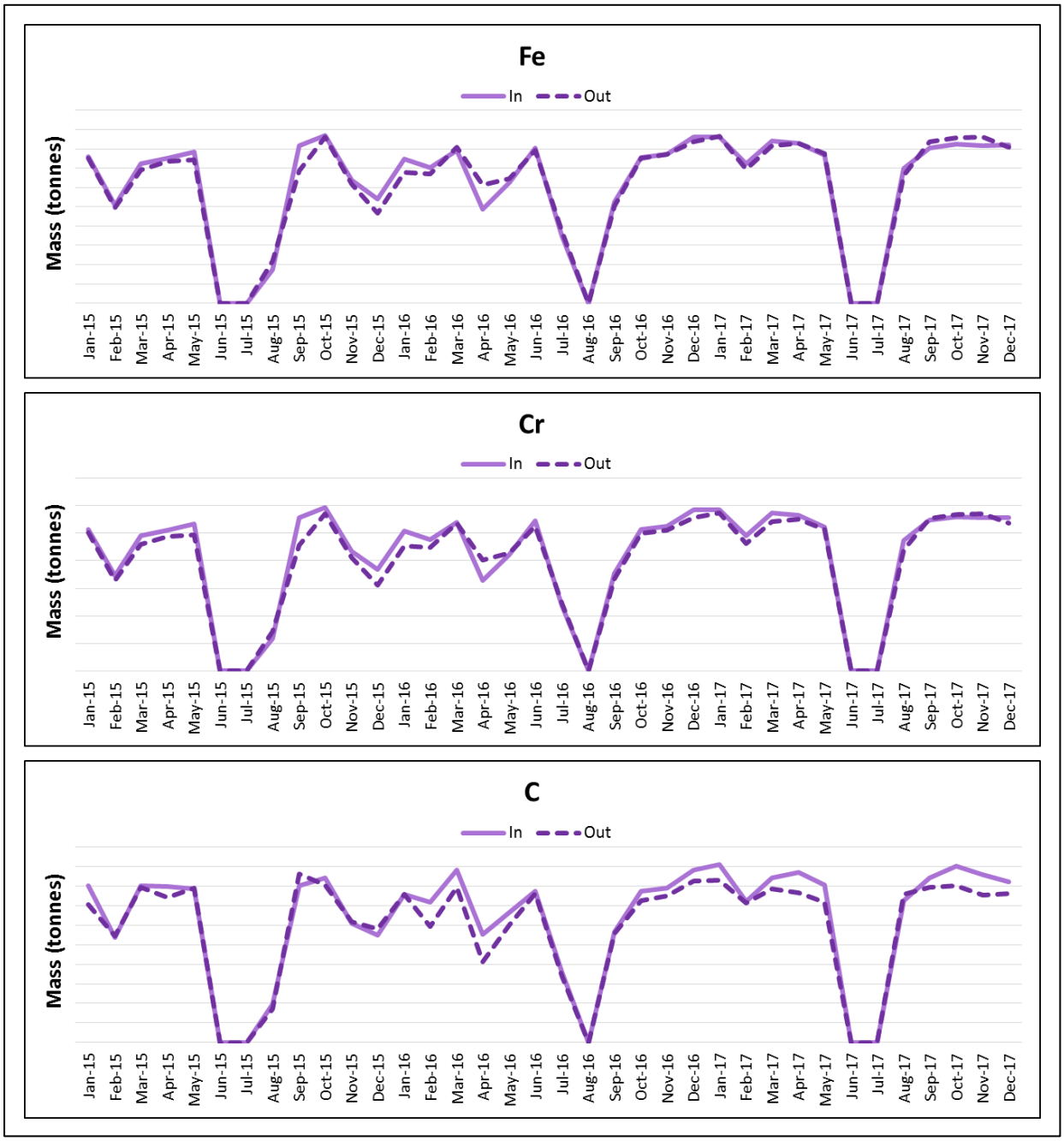


Figure 3-25: Elemental (Fe, Cr, C) mass balance trends (CS2)

Once the elemental mass of all streams are known, Equation 3-17 can be derived to perform a mass balance on every element present in the furnace in order to calculate the error of the mass balance (*step 6*). This is done to verify the total CO_2 emissions calculated for 2017: 117 496 tonnes (*step 5*). Equation 3-20 and Equation 3-21 are applied, and the results are shown in Table 3-17.

Table 3-17: Total elemental balance error results (CS2)

	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Total X_in	39 897	54 317	15 401	41 567	16 365	84 637	4 960	13 552	1 859	958	522	13 990
Total X_out	40 038	53 141	19 100	38 412	16 437	94 185	4 240	13 835	429	3 686	314	4 187
Error (%)	0%	2%	24%	8%	0%	11%	15%	2%	77%	285%	40%	70%
Total elemental balance error (%)	**0.0%**	**0.4%**	**1.3%**	**1.1%**	**0.0%**	**3.3%**	**0.2%**	**0.1%**	**0.5%**	**0.9%**	**0.1%**	**3.4%**

The total mass balance error is calculated as 11.4% (sum of all "total elemental balance errors"), meaning that the total CO_2 emissions = 117 496 tonnes ± 11.4% = 117 496 tonnes ± 13 446 tonnes.

CS2 summary

This case study was based on measurements from site. The slag mass was assumed to be correctly estimated on site, after which the off-gas mass was determined. After this, the mass of each element entering and exiting the furnace could be calculated before the total elemental balance error was quantified. The CO_2 emissions were calculated to be 117 496 tonnes ± 13 446 tonnes, with an error of 11.4%. These results show a significant improvement from the previous case study, where a mass balance error of 19.9% was found.

More details regarding this case study can be found in Appendix F.

3.4.5 Case study 3: Advanced mass balance

Where the previous two case studies were based on assumptions from literature, or actual measurements from site, the CS3 will require more intuitive engineering applications, which will be based on FeCr knowledge obtained throughout this study.

For *step 1*, a slag mass must be determined before the overall mass balance can be constructed to calculate the mass of the off-gas exiting the furnace (*step 2*). This will be done by assuming that the compound Al_2O_3 doesn't react during the FeCr production process (explained in detail in Section 3.3.7, sub-section: "*Advanced mass balance*"). According to the data from site (dataset "c"), the slag contains 28.53% Al_2O_3. The slag mass can thus be calculated by applying Equation 3-22. Next, the off-gas mass can be estimated by performing an overall balance (Equation 3-16).

Since the off-gas is the only unmeasured stream regarding composition (Table 3-14), *step 3 and 4* allow for an elemental balance to quantify the off-gas composition (*step 5*). Equation 3-17 is applied to the elements present within the off-gas. The following results are obtained (Table 3-18).

Table 3-18: Off-gas composition analysis (CS3)

Stream	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Off-gas	**-**	**-**	**-**	**40.3**	**-**	**45.3**	**-**	**-**	**2.1**	**1.1**	**0.2**	**11.0**

Since the C-content is the most important element when estimating CO_2 emissions, the calculated content will be verified by off-gas composition analysis range from literature. Table 3-1 (Section 3.2.2) gives the typical carbon content in FeCr furnace off-gas as 28%-44%. These are set as upper- and lower limits and compared to the newly calculated C-content, which is shown in Figure 3-26. It is clear that the calculated C-content falls within the limits given by literature.

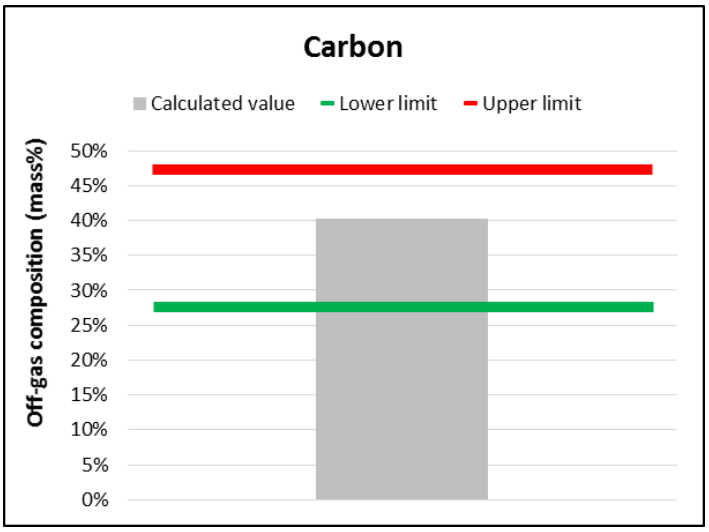


Figure 3-26: Off-gas elements with upper and lower limits from literature (CS3)

Once the elemental mass of all streams are known, Equation 3-17 can be derived to perform a mass balance on every element present within the furnace to calculate the error of the mass balance (*step 6*). This is done to verify the total CO_2 emissions calculated for 2017: 129 063 tonnes. After Equation 3-20 and Equation 3-21 are applied, the elemental balance error results are obtained and provided in Table 3-19.

Table 3-19: Total elemental balance error results (CS3)

	Fe	Cr	Si	C	Al	O	Ca	Mg	H	N	S	Trace
Total X_in	39 897	54 317	15 401	41 567	16 365	84 637	4 960	13 552	1 859	958	522	13 990
Total X_out	40 021	53 112	19 035	41 567	16 365	84 637	4 221	13 775	1 859	958	522	13 990
Error (%)	0%	2%	24%	0%	0%	0%	15%	2%	0%	0%	0%	0%
Total elemental balance error (%)	**0.0%**	**0.4%**	**1.3%**	**0.0%**	**0.0%**	**0.0%**	**0.3%**	**0.1%**	**0.0%**	**0.0%**	**0.0%**	**0.0%**

The total mass balance error is calculated as 2.1% (sum of all "total elemental balance errors"), meaning that the total CO_2 emissions = 129 063 tonnes ± 2.1% = 129 063 tonnes ± 2 654 tonnes.

CS3 summary

This case study was based on a more advanced approach based on FeCr furnace knowledge. The slag mass was determined by assuming certain FeCr furnace characteristics, after which the off-gas mass was determined. After this, the composition of the off-gas was estimated and compared to literature. All elements entering and exiting the furnace were calculated before the total elemental balance error was quantified. The CO_2 emissions were calculated to be 129 063 tonnes ± 2 654 tonnes, having a mass balance error of 2.1%. These results show a significant improvement from the previous case study, where a mass balance error of 11.4% was found.

More details regarding this case study can be found in Appendix F.

3.4.6 Case study summary

The main goal of this section was to verify the methodology developed in Section 3.3, which aimed to calculate the CO_2 emissions from the furnace in the most accurate way possible. Three detailed case studies (CS) were used to showcase each one of the three stages of mass balance development: CS1) *literature* mass balance (Section 3.4.3), CS2) *measured* mass balance (Section 3.4.4), and CS3) *advanced* mass balance (Section 3.4.5). The results obtained from these case studies are provided in Table 3-20:

Table 3-20: Verification summary – refining prescribed methods

Result	**Case study 1** (*Literature MB*)	**Case study 2** (*Measured MB*)	**Case study 3** (*Advanced MB*)
CO_2 emissions (tonnes)	76 057 tonnes	117 496 tonnes	129 063 tonnes
Mass balance error (%)	19.9%	11.4%	2.1%

These case studies illustrated that each stage of mass balance calculation was an improvement on the previous (19.9% error > 11.4% error > 2.1% error). It is evident that just using literature composition values will not provide reliable results (19.9% error). Only once the measured values are used in combination with certain assumptions based on FeCr characteristics, one may achieve better results (smallest mass balance error, 2.1%). Therefore, the CO_2 emissions result from the advanced mass balance is the most trustworthy (129 063 tonnes). A visual representation of each case study's results are shown in Figure 3-27, where the black bars show the error margins.

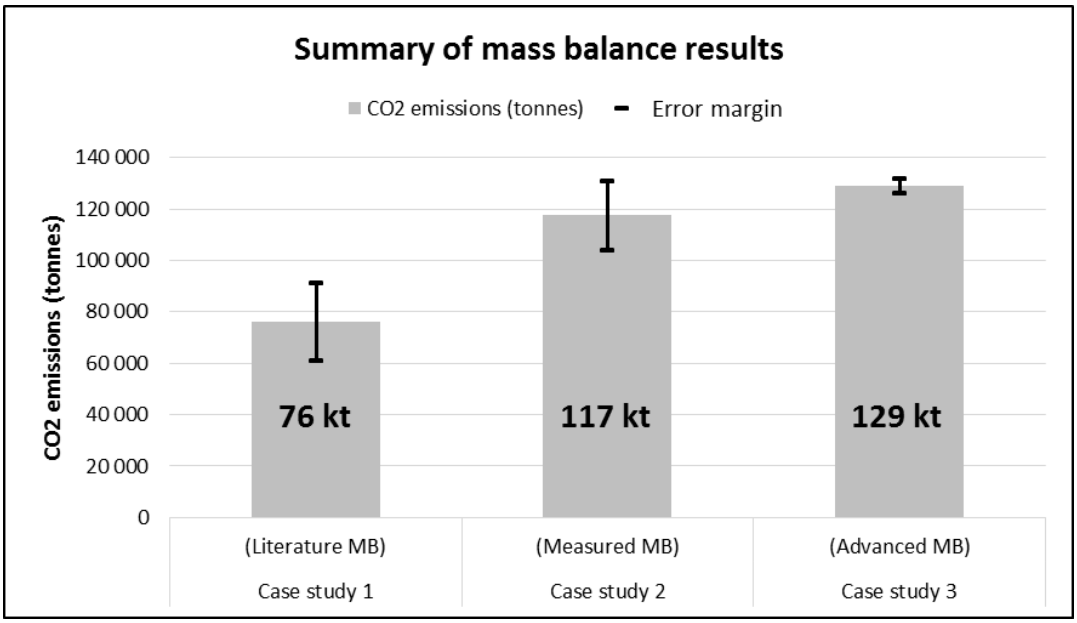


Figure 3-27: Summary of mass balance results

Even though each case study's CO_2 emission results differ significantly, the results of the *advanced mass balance* (CS3) are the most trustworthy, due to the smaller error margin. This section used one furnace (Furnace X) for all three case studies. In addition to this, 16 other furnaces were investigated, and similar case studies were done. These results can be seen in Appendix E.

3.5 Conclusion

It was found that the three prescribed methods to quantify CO_2 emissions from FeCr production are not necessarily accurate and may also vary significantly from one another (Section 2.4). The need was therefore established to refine these prescribed methods into a more complex, yet accurate approach. This section used the construction of mass balances to explore the idea of refining the tier 3 approach.

The elements present within the streams entering and exiting a FeCr furnace were revised, which led to a new approach on estimating the total elemental composition (TEC) of reductants. A brief discussion on relevant statistical concepts was then provided, before researching some background information on mass balances and the construction thereof.

The methodology was then developed to be used when constructing the refined mass balances. Verification of the methodology took place in Section 3.4, where three case studies were used to illustrate each stage of the methodology. These case studies proved that by constructing an

advanced mass balance, a much smaller error will be achieved, adding to the reliability of the final results.

The question of whether the method of advanced mass balances are 'better' than performing a prescribed method (tier 1, 2, or 3) are still up for discussion. Is it worthwhile to go through all the effort of constructing detailed mass balances, when only a simple tier 1 equation could have been used? The next chapter will focus on bringing together all case studies done throughout the study, and comparing the results. The balancing of accuracy versus complexity will also be addressed.

4. COMPARISON OF DIFFERENT METHODS

4.1. Introduction

This study started out with the FeCr industry and the fact that carbon tax is becoming a reality. To estimate the carbon tax liability of a certain entity, the CO_2 emissions must be determined as accurately as possible. After a comprehensive literature study was done, the conclusion could be drawn that, although there are prescribed formulas that exist to perform these calculations, there was a lack of literature studying the practical application of these methods, as well as the implications associated. This led to the aim of the study.

Chapter 2 therefore evaluated the three prescribed calculation methods in terms of the practical applicability. It became clear that, even though these formulas were relatively simple, the practical application is risky and sensitive to errors in data and general understanding of how the system works. This chapter ended with the three prescribed methods delivering different results, together with possible constraints that may cause the results to vary even more.

According to literature, tier 3 is the most accurate of the three prescribed methods, and is based on a mass balance approach. In Chapter 3, it was decided to use the concept of tier 3 (construction of mass balances) to explore the idea of refining the prescribed methods. After more accurate results were achieved, the following question arose: is it worthwhile to go through all the effort of constructing detailed mass balances, when only a simple tier 1 equation could have been used?

This chapter will focus on bringing together the six quantification methods (tier 1, tier 2, tier 3, mass balance 1, mass balance 2, and mass balance 3) from the case studies done throughout the study, and comparing the results. Section 4.2 will give the comparison of the different methods and the variance that exists between them.

In Section 4.3, the accuracy and the complexity of different methods will be discussed (Sections 4.3.1 and 4.3.2, respectively), and will then be compared to one another in Section 4.3.3. The chapter will be concluded in Section 4.4. Figure 4-1 shows the outline of this chapter (next page).

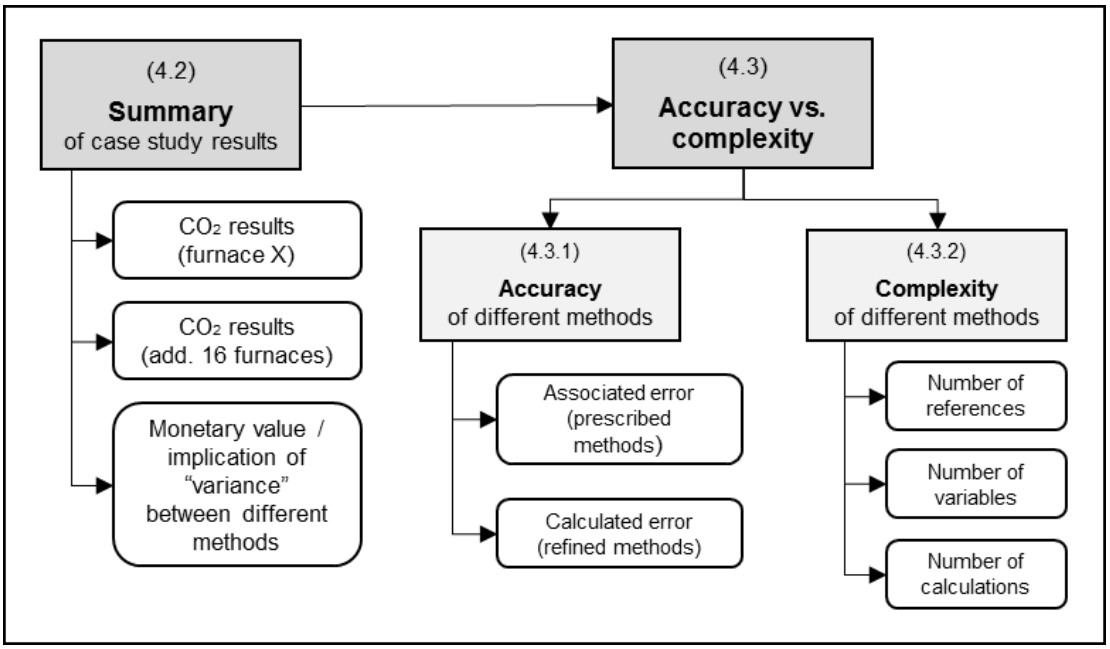


Figure 4-1: Approach to compare the different CO_2 emission quantification methods

4.2. Summary of case study results

Throughout the course of this study, different methods were investigated to quantify the CO_2 emissions (tonnes) from a FeCr furnace. This was done with the aim to estimate the carbon tax monetary liability, which is calculated by multiplying the CO_2 emissions with the carbon tax rate (R120 per tonne CO_2). Table 4-1 provides the six CO_2 quantification methods investigated throughout the study, the relevant chapters where they were discussed, and an abbreviation for each to simplify reference further on.

Table 4-1: Six CO_2 quantification methods investigated

Chapter	Quantification method	Description	Abbreviation used in Chapter 4
Chapter 2 (prescribed methods)	Tier 1	Production-based emission factors	T1
	Tier 2	Production-based, raw material-specific emission factors	T2
	Tier 3	Calculations based on amounts and analyses of reducing agents	T3
Chapter 3 (refined mass balance methods)	Literature	Mass balance based on literature	MB1
	Measurements	Mass balance based on measurements	MB2
	Advanced	Mass balance based on furnace characteristics	MB3

Furnace X was used for illustrating the case studies in Chapter 2 and 3. In Chapter 2, three case studies were used to highlight the significance of certain areas in the methodology. Tier 1, 2 and 3

were used, and the results of these case studies showed that less accurate results may be obtained if the correct procedure is not followed. The final CO_2 quantities calculated by the three different methods were 124 059 tonnes (T1), 136 737 tonnes (T2), and 150 733 tonnes (T3).

In Chapter 3, three case studies were used to showcase each one of the three stages of the mass balance development. These case studies gave the following results: 76 057 tonnes (MB1), 117 496 tonnes (MB2), and 129 063 tonnes (MB3). The CO_2 emission results for Furnace X (quantified by six different methods/approaches) are compared in Figure 4-2.

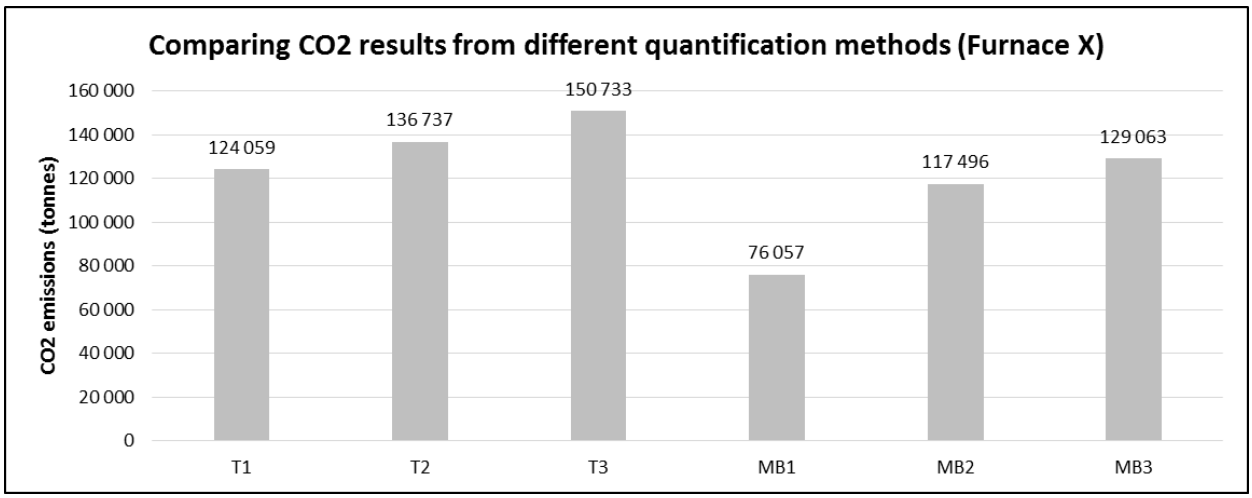


Figure 4-2: Comparison of CO_2 emission results for Furnace X

It is clear that the different methods give varying results, as suspected in Chapter 1, ranging from 76 057 tonnes to 150 733 tonnes CO_2. This significant variance is quantified by two different approaches, including the *range method* (difference between the minimum value and the maximum value) and the *standard deviation* (concentration of the data around the mean of the dataset). The standard deviation is used in addition to the range approach to consider the rest of the data values as well, and not just the minimum and maximum values. This will allow for a certain exclusion of the influence of outliers. The results for these are given below in Equation 4-1 and Equation 4-2:

$$Range(\%) = \frac{max - min}{max} = \frac{150\,733 - 76\,057}{150\,733} = \mathbf{50}\%\ variance$$

Equation 4-1: Data range (%)

$$\sigma = \frac{\sqrt{\frac{\sum(x - \bar{x})^2}{n}}}{\bar{x}} = \frac{\sqrt{\frac{3\,227\,188\,764}{6}}}{122\,357} = \mathbf{19}\%\ variance$$

Equation 4-2: Standard deviation (%)

Both these values are given as percentages (%) so that it can be compared objectively with other furnaces.

The data range is quantified as 50%, and the standard deviation as 19%. This means that the CO_2 emissions calculated for Furnace X have a variance of 19-50%. The quantification of these ranges is repeated for the additional 16 furnaces referred to at the end of Chapters 2 and 3 (where the case studies were repeated in Appendix E and G). The variance results of the different furnaces are shown in Figure 4-3, where the data range and standard deviation results are represented by the light grey- and dark grey bars, respectively.

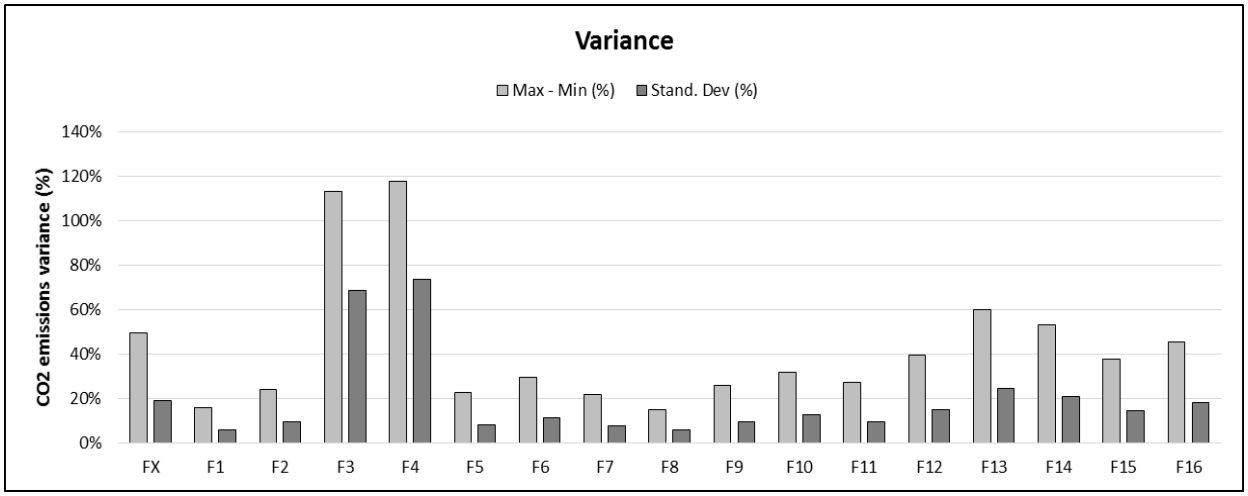


Figure 4-3: Comparison of CO_2 emission ranges for furnace X and furnace 1 - 16

The variances for furnace 3 (F3) and furnace 4 (F4) are clearly higher than that of the other furnaces. It is important to know that these two are direct current (DC) furnaces, where the rest are all alternating current (AC) furnaces. A difference between the two is that the DC furnace can handle the use of finer feed material without the need to agglomerate by means of briquetting or pelletising. The raw feed of DC furnaces also vary significantly from AC furnaces, which has a big impact on the process [65, 151]. Due to the fundamental difference between these two types of furnaces, F3 and F4 are excluded from the group for any further calculations and comparisons.

One of the concerns highlighted in Chapter 1 underlined the following question: *How would the different furnace technologies influence the emissions?* (Question E). The discussion in the previous paragraph shows that different furnace technologies will indeed have an influence on the final results. Unfortunately there is not sufficient information and data to evaluate and address this concern, which is why it will be regarded as one of the future recommendations (Chapter 5).

To summarise the final uncertainty of the different CO_2 emission quantification methods from a FeCr furnace, the average of the variances from the 15 different furnaces (excluding F3 and F4) were calculated, and found to be 33% (range method) and 13% (standard deviation). This means

that the CO_2 emissions calculated for 15 South African FeCr furnaces have a variance of 13-33%, which is illustrated by Figure 4-4 (elaboration of Figure 4-3).

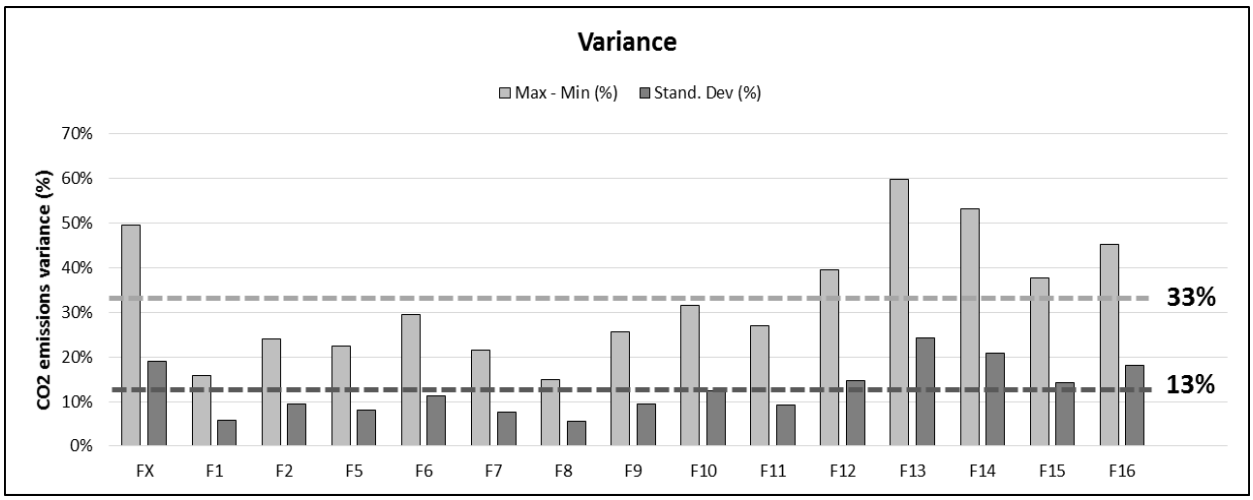


Figure 4-4: Estimation of average CO_2 emission ranges for furnace X and furnace 1 - 16

This average variance can now be translated into a monetary value to estimate the associated risk. The following figure is taken from Chapter 1 (Section 1.1), where the generation of off-gas volumes from the ferroalloy production industry is illustrated (Figure 4-5).

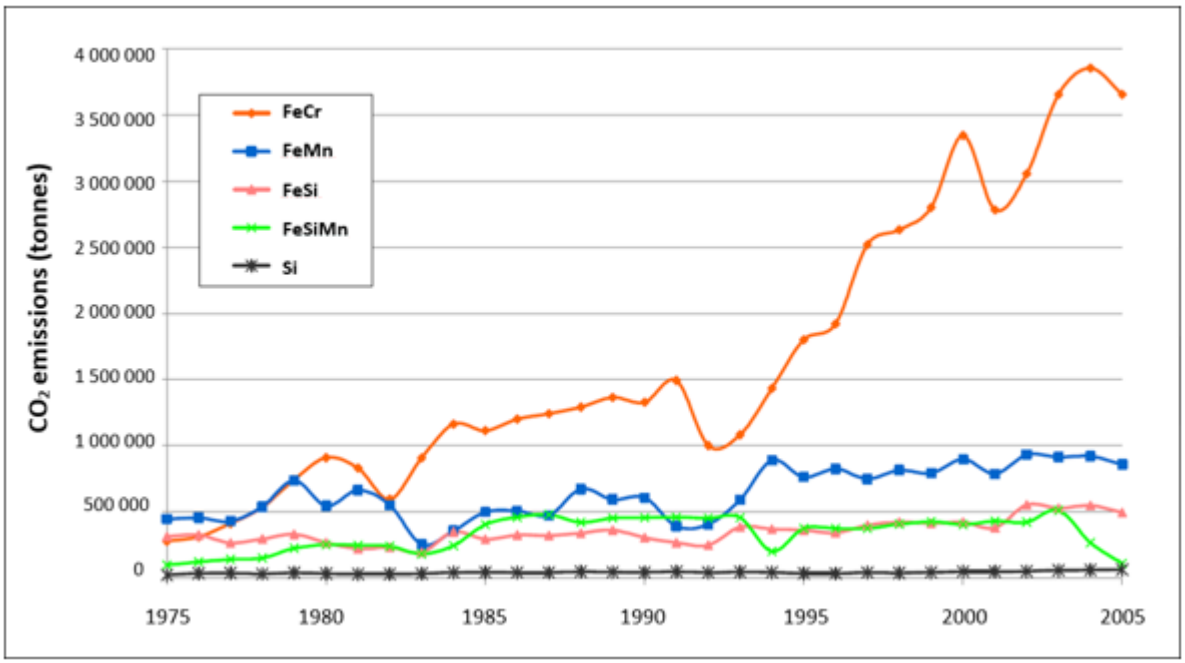


Figure 4-5: GHG emissions from ferroalloy production in SA (repeat of Figure 1-2)

The total CO_2 emission estimation from FeCr production (orange line in graph) was approximately 3.6 Mt for 2005 [27]. Due to the increase of FeCr production (± 30% from 2005 to date [28, 29]), it was assumed that CO_2 emissions from FeCr production increased with the same percentage: 3.6×10^6 tonnes + 30% = **4.68×10^6 tonnes CO_2** per year (2017 estimate).

The estimated carbon tax liability is thus R562 million per year (4.68×10^6 tonnes CO_2 × R120 per tonne CO_2), of which the average variance/uncertainty range due to different calculation methods is 13-33%, i.e. R562 million ± R75-R185 million per year. This is a significant amount, which is why it is important to investigate the associated error of each CO_2 quantification methods.

Another way used to visualise the comparison between the different methods is given by Figure 4-6. This figure shows the total amount of CO_2 emissions against the total FeCr production (both in tonnes) for the six different quantification methods.

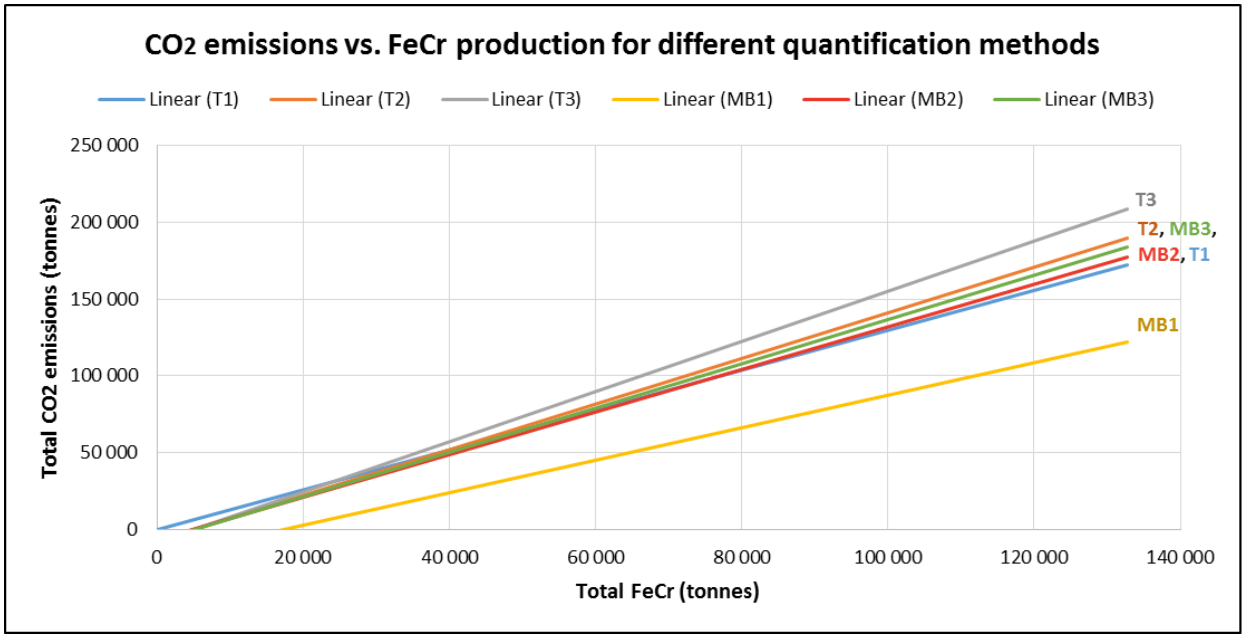


Figure 4-6: CO_2 emissions vs FeCr production for different quantification methods

The primary visual observation that can be made from Figure 4-6 is the two outlier lines, T3 (grey) and MB1 (yellow). According to this figure, T3 gives the highest results of all the methods. It is also expected to give the most accurate results (according to literature). However, this doesn't seem likely, as the majority of the lines lie in a cluster below T3. MB1 gives very low results. It is found that this method is very sensitive for the selection of assumed literature values, e.g. slag-to-metal ratio. Since T1, T2, MB2, MB3 all lie close together, it is most probable that the true result is in this region.

This section showed that there are clear and significant discrepancies between the different emission quantification methods, thus confirming the relevance of this study. It is necessary to critically evaluate the accuracy and the complexity of the different methods to evaluate whether it will be worthwhile to do more intricate and complex calculations (such as MB3) to acquire more accurate results. Section 4.3 will discuss these two concepts and compare them.

4.3. Accuracy vs. complexity

4.3.1 Accuracy

Accuracy refers to the closeness of a measured value to a known or standard value.[5] Since the errors or uncertainties were reported or calculated for the six different methods, this needs to be translated to an accuracy value. A simple calculation is used to do this conversion (Equation 4-3):

$$Accuracy\ (\%) = 100\% - Error(\%)$$ *Equation 4-3: Error-to-accuracy conversion*

All errors discussed in this section will eventually be converted to an associated accuracy in Section 4.3.3, where the accuracy and complexity will be compared.

The reported errors/uncertainties of the prescribed methods, T1, T2 and T3, are 25% - 50%, ±10% and <5%, respectively [35]. Since these reported errors do not change with the application to different furnaces, only the mass balances (MB1, MB2 and MB3) will be investigated in terms of their errors for each individual furnace. The following figure shows the associated errors for 15 SA FeCr furnaces according to MB1, MB2 and MB3, which are indicated by the black-, dark grey- and light grey bars, respectively. The calculation of these errors can be found in Appendix E.

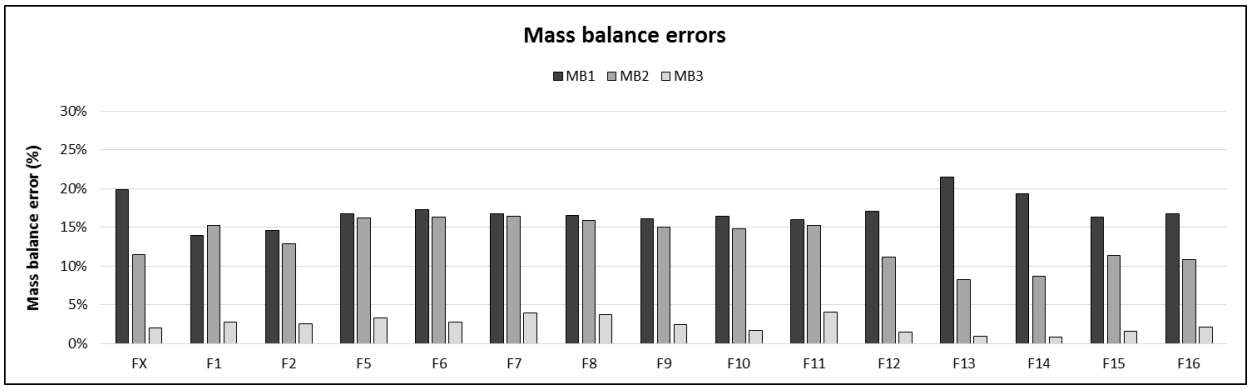


Figure 4-7: Errors associated with three stages of mass balances for 15 furnaces

From Figure 4-7, it is clear that, on average, the error of MB1 is greater than that of MB2. The MB2 errors are also greater than the MB3 errors, which are 2.4% on average, i.e. MB1 error > MB2 error > MB3 error. This implies that the *advanced mass balance* (MB3) shows the most accurate results of all CO_2 quantification methods. Table 4-2 provides a summary of the average error associated with each quantification method:

[5] https://labwrite.ncsu.edu/Experimental%20Design/accuracyprecision.htm

Table 4-2: Average errors associated with each quantification method

Quantification method	Average associated error	Reference
T1	25-50%	IPCC [35]
T2	±10%	IPCC [35]
T3	<5%	IPCC [35]
MB1	17.0%	Calculation [Appendix H]
MB2	13.3%	Calculation [Appendix H]
MB3	2.4%	Calculation [Appendix H]

It should be noted that T3 is a very basic mass balance, prescribed by the IPCC. MB1, 2, and 3 are methods to refine this simple mass balance approach, which is T3, as discussed in Chapter 3. It can be seen that, according to the literature (IPCC), a mass balance approach is supposed to give an estimated error of <5%. It is found, however, that T3 is very sensitive, i.e. MB1-3 are all mass balances based on T3, but have errors ranging from 2.4% to 17.0%.

It is clear that literature-based mass balances would not give an error of <5%, as suggested by IPCC, but as soon as more detail is brought into this mass balance and specific furnace characteristics are considered, this small error (<5%) may be achieved. This confirms the problem highlighted by the critical literature review: since carbon tax has not been implemented, it is not yet fully understood and no practical examples on how to apply different methods are available.

From the results in this section, MB3 gives the smallest error. There is a concern, however, that this quantification method is too complex, and consumes too much time to perform. There is a need to investigate and compare the complexity and accuracy of these different methods (prescribed and developed), i.e. is it worthwhile to go through these complex calculations (MB3) to get a relative accurate result? The complexity aspect will be discussed in the next section, whereafter the complexity and accuracy will be compared.

4.3.2 Complexity

Some of the CO_2 quantification methods require more complex applications than others. Where Tier 1 only requires the amount of FeCr produced and a production emission factor provided by the IPCC, some of the mass balances would require many complex calculations, assumptions and interpretations. To compare the different quantification methods objectively in terms of the complexity, three factors are considered, namely the number of references, the number of variables and the number of calculations. A discussion of each of these aspects follows.

Number of references

Each method uses certain references to calculate the total CO_2 emissions from the FeCr furnace. The following list describes the references used by each method:

- T1 uses one reference only (IPCC), where the equation and the emission factor are given [35].
- The equation for T2 is also referenced from the IPCC [35]. In addition to this, the carbon contents of the following materials are obtained: dolomite [126], limestone [127], quartz: [128], and FeCr product [7]. The emission factors of reductants are also obtained through two different sources [118, 119].
- T3 uses the same references as T2 [7, 35, 126, 127, 128]. However, instead of emission factors of reductants being used, the carbon content is used: char: [124], coke [125], coal [123].
- MB1 uses the compositions of all materials entering and exiting the furnace: ore [7], dolomite [126], limestone [127], quartz [128], FeCr product [7], slag [77], char [124], coke [125], coal [123]), off-gas [15, 14]. In addition to this, a slag ratio from literature is assumed [130].
- Since the compositions of slag and FeCr product are usually known from site, MB2 only uses references for the compositions of the following materials: ore [7], dolomite [126], limestone [127], quartz [128], and off-gas [15, 14]. Also, the TEC of the reductants are calculated, based on assumptions from the following references: [133, 134, 135, 136, 138].
- MB3 uses similar references as MB2, except that in this case, the off-gas composition is calculated and not assumed from literature. An advanced assumption is made, however, to calculate the slag mass [149, 150].

This is summarised in Table 4-3 below, where the total number of references used are provided.

Table 4-3: Number of references used per quantification method

Quantification method	References used	Number of references used
T1	[35]	1
T2	[35, 7, 126, 127, 128, 118, 119]	7
T3	[35, 7, 126, 127, 128, 123, 124, 125]	8
MB1	[7, 126, 127, 128, 123, 124, 125, 14, 15, 77] [130]	11
MB2	[7, 126, 127, 128, 14, 15, 77, 133, 134, 135] [136, 138]	12
MB3	[7, 126, 127, 128, 77, 133, 134, 135] [136, 138, 149, 150]	12

Number of variables used

Each method uses a certain number of variables to calculate the total CO_2 emissions from the FeCr furnace. The following table indicates the variables required by each method:

Table 4-4: Number of variables used per quantification method

Variable used in method	T1	T2	T3	MB1	MB2	MB3
Mass: FeCr ore		1	1	1	1	1
Mass: Reductant (coal)		1	1	1	1	1
Mass: Reductant (coke)		1	1	1	1	1
Mass: Reductant (char)		1	1	1	1	1
Mass: Flux (limestone)		1	1	1	1	1
Mass: Flux (dolomite)		1	1	1	1	1
Mass: Flux (quartz)		1	1	1	1	1
Mass: FeCr product	1	1	1	1	1	1
Mass: Slag product		1	1		1	
Carbon content: Reductant (coal) - 1 element			1			
Carbon content: Reductant (coke) - 1 element			1			
Carbon content: Reductant (char) - 1 element			1			
Carbon content: Flux (limestone) - 1 element		1	1			
Carbon content: Flux (dolomite) - 1 element		1	1			
Carbon content: FeCr product - 1 element		1	1			
Composition: FeCr ore – 7 elements				7	7	7
Composition: Reductant (coal) – 5 elements				5	5	5
Composition: Reductant (coke) - 5 elements				5	5	5
Composition: Reductant (char) - 5 elements				5	5	5
Composition: Flux (limestone) - 3 elements				3	3	3
Composition: Flux (dolomite) - 4 elements				4	4	4
Composition: Flux (quartz) - 2 elements				2	2	2
Composition: FeCr product - 4 elements				4	4	4
Composition: Slag product - 7 elements				7	7	7
Composition: Off-gas - 4 elements				4	4	
Composition: Al_2O_3 (slag, ore, dolomite, limestone, quartz)						5
Emission factor (production)	1					
Emission factor (coal)		1				
Emission factor (coke)		1				
Emission factor (char)		1				
Slag:metal ratio				1		
Total variables	**2**	**15**	**15**	**55**	**55**	**55**

Number of calculations used

Each method uses a certain number of calculations to quantify the total CO_2 emissions from a FeCr furnace. Since the calculations for T1, T2 and T3 are all given in the IPCC as a single equation, these methods only make use of one calculation. As for the mass balances, the following table provides the equations used for MB1, MB2 and MB3. However, this is irrespective of how many times it is utilised.

Table 4-5: Number of variables used per quantification method

Equations used in method	T1	T2	T3	MB 1	MB 2	MB 3
Equation 1-3: Calculation method - Tier 1	1					
Equation 1-4: Calculation method - Tier 2		1				
Equation 1-5: Calculation method - Tier 3			1			
Equation 3-7: Determining the total content of element X in coal				1	1	1
Equation 3-8: TEC of coal (C)					1	1
Equation 3-9: TEC of coal (H)					1	1
Equation 3-10: TEC of coal (O)					1	1
Equation 3-11: TEC of coal (N)					1	1
Equation 3-12: TEC of coal (S)					1	1
Equation 3-13: TEC of coal (trace)					1	1
Equation 3-14: Mean (or average) value				1	1	1
Equation 3-15: Standard deviation				1	1	1
Equation 3-16: Overall mass balance				1	1	1
Equation 3-17: Elemental mass balance				1	1	1
Equation 3-18: Determining mass of element X in material Y				1	1	1
Equation 3-19: Determining slag mass with slag:metal ratio				1		
Equation 3-21: Total elemental balance error				1	1	1
Equation 3-22: Slag mass estimation from Al_2O_3						1
Equation X: Determining off-gas composition						1
Equation B-1: Molecular weight of material "d"				1	1	1
Equation B-2: Composition - amount of element ("x") present in material ("d")				1	1	1
Total number of calculations	**1**	**1**	**1**	**10**	**15**	**17**

Complexity summary

The three complexity factors are added up to obtain a final quantified complexity value for each quantification method. This can be seen in Table 4-6.

Table 4-6: Factors of complexity associated with each quantification method

Quantification method	Number of references used	Number of variables used	Number of calculations used	Final quantified complexity
T1	1	2	1	**4**
T2	7	15	1	**23**
T3	8	15	1	**24**
MB1	11	55	10	**76**
MB2	12	55	15	**82**
MB3	12	55	17	**84**

These results are illustrated visually in Figure 4-8.

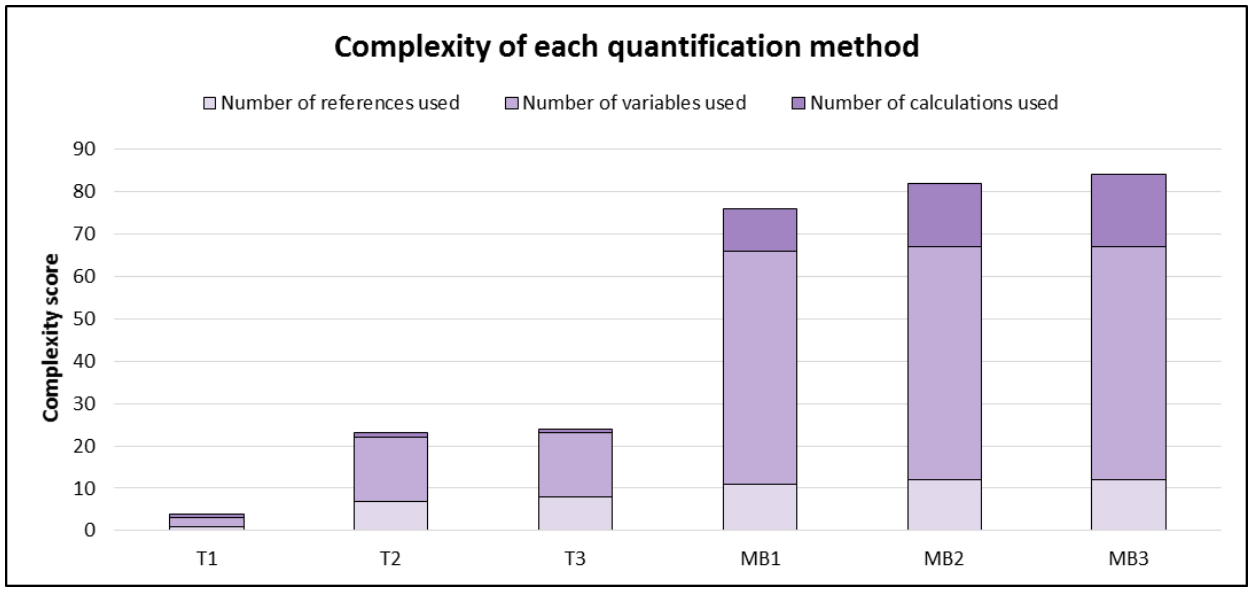


Figure 4-8: Complexity associated with each quantification method

Figure 4-8 shows a significant difference in the complexity between T1 and T2, where T2 and T3 are rather similar. However, as soon as the prescribed methods are refined, the complexity increases tremendously, growing with approximately 210% (complexity score of 24 to 76). Hence, the refined methods (MB1, MB2 and MB3) require much more work, and are more complex.

4.3.3 Summary

The following question arose throughout the evaluation of this study: is it worthwhile to go through all the effort of constructing detailed mass balances, when only a simple tier 1 equation could have been used? The accuracy and complexity of the different methods were discussed and calculated and combined in Figure 4-9. Note that the accuracy of the methods are calculated as 100% - error (from Table 4-2).

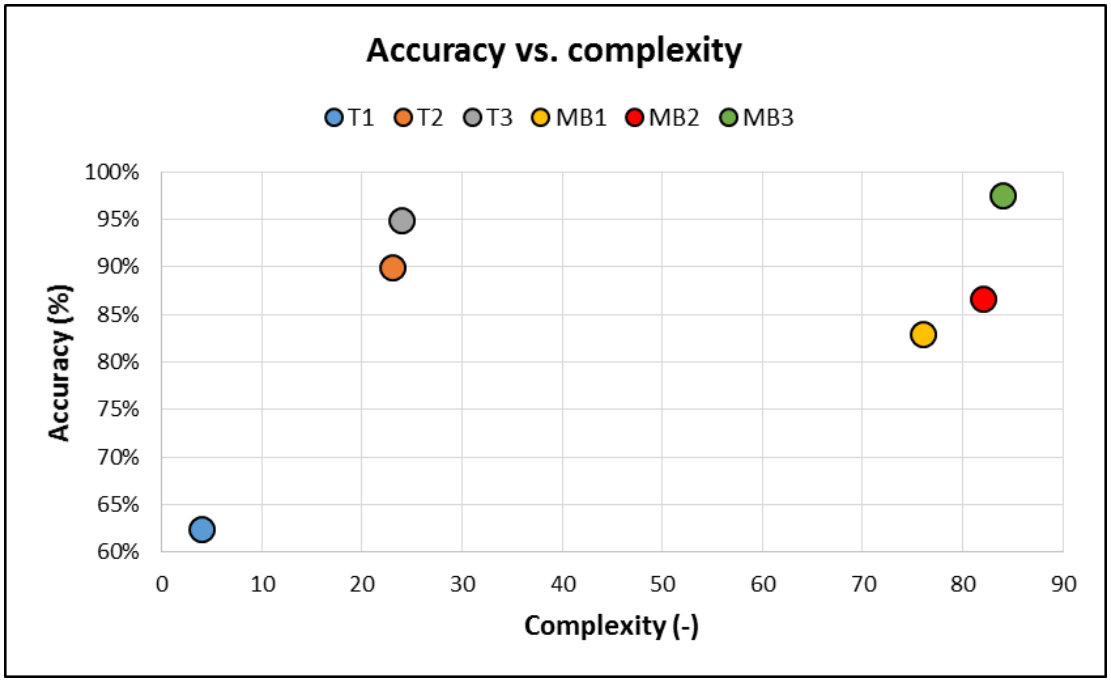


Figure 4-9: Accuracy vs. complexity of each quantification method

Figure 4-9 illustrates that the T1 method (blue dot) requires the least amount of work (low complexity), but also generally delivers low accuracy. Since the accuracy of the prescribed methods are suggested by literature, and not specifically calculated, the plotted positions of T1, T2 and T3 plotted are seen as estimations only. For the three mass balances (MB1, MB2 and MB3), it is seen that a better accuracy can be achieved if more complexity is added. Based on this observation, it is confirmed that it is worthwhile to go through the effort of constructing a detailed mass balance, rather than using a simple T1 method.

When only the two extremes are used to illustrate the potential carbon tax liability for the 15 evaluated furnaces, the use of method T1 (lowest complexity, lowest accuracy) would result in an annual liability of R258 million ± R97 million, whereas MB3 (highest complexity, highest accuracy) would give a value of R219 million ± R5 million. Note that this is for the 15 furnaces evaluated, which make up approximately 50% of the FeCr industry in SA, which is why both these values make up approximately half of the original quantified CT liability of R562 million.

Figure 1-5 from Chapter 1 illustrated how the complexity and the uncertainty of the different prescribed methods vary. This figure is repeated in Figure 4-10.

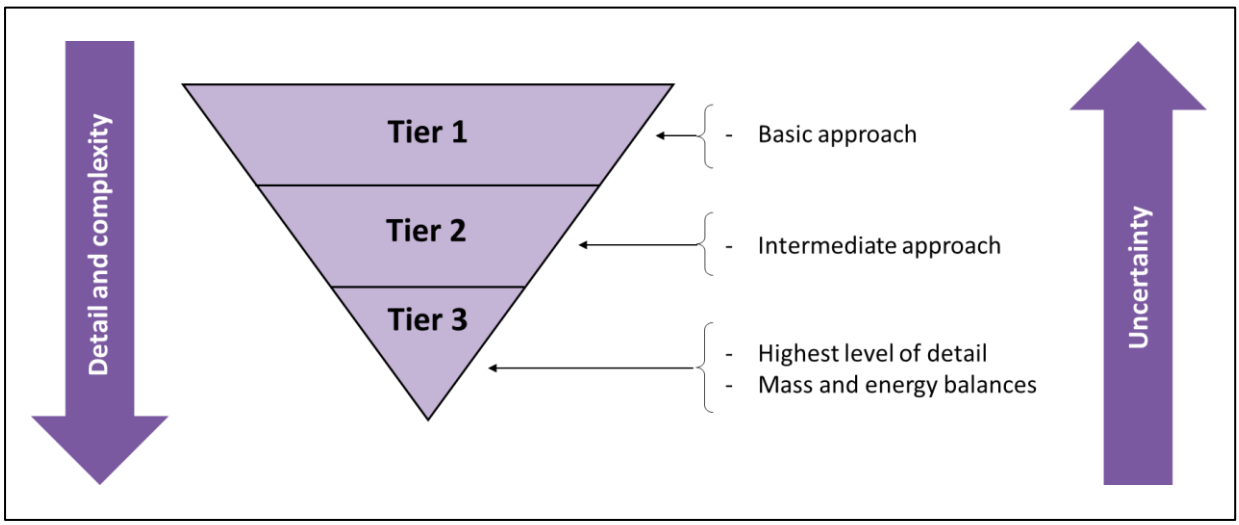


Figure 4-10: Comparative structure of prescribed tiers (repeat of Figure 1-5)

According to this figure, T1 is the most basic approach, with the highest level of uncertainty. T2 requires more detail than T1, while T3 is the most complex method of all, having the lowest uncertainty (highest accuracy). This confirms what is found by the calculations and comparisons done in Chapter 4 and illustrated in Figure 4-9.

4.4. Conclusion

The application of the different quantification methods gave a variance of 13-33% on the calculated CO_2 emission result. This translates to a variance of R75 million – R185 million (R562 million ± R75-R185 million) per year in carbon tax liability, for the entire SA FeCr industry, just due to the use of different methods. Hereafter, the accuracy of the different methods were compared. According to literature, tier 1 is less accurate (25%-50% error) and tier 3 more accurate (<5% error). However, if this is implemented practically, it is evident that this small error (<5%) is only achievable when tier 3 is done thoroughly, as with mass balance 3.

The complexity of the different methods increase significantly between the prescribed methods and the refined mass balances. It was found, however, that with a little extra “complexity” a much higher accuracy can be accomplished by going from mass balance 2 to mass balance 3. Based on the method developed throughout this study, and based on the case studies performed, MB3 gives an average error of 2.4% and a final quantified complexity of 84 (highest of all methods).

5. CONCLUSION

5.1. Summary of work

Ferrochrome furnaces are significant CO_2 emitters due to the large amounts of carbon-containing materials being used. FeCr industries will therefore become liable for carbon tax (CT), which is to be implemented soon. These industries will thus have to pay CT eventually. However, the way to quantify the CO_2 emissions is overly generic and the implementation thereof still uncertain. This study was conducted to critically assess the CO_2 emission quantification methods in the ferrochrome industry. This must be done in order to ultimately calculate the monetary CT liability.

FeCr industries in SA may be liable for ±R562 million per year (original quantification based on literature only), which proves that the uncertainties around emission quantification for the FeCr industry is a significant concern. This problem was broken down into three smaller problems, which was addressed throughout the document.

Chapter 1 provided relevant background information on FeCr furnaces and the associated emissions. Some uncertainties were identified in the form of research questions, which lead to an in-depth critical literature review, whereafter certain gaps were identified. The gaps became the three focus areas of the study, and were discussed and addressed in Chapters 2, 3 and 4.

Chapter 2 highlighted the problem of how carbon tax is not yet fully understood, and how no sufficient practical examples of the application of different methods are available. The need to illustrate the application of these methods was therefore addressed and assessed in terms of the simplicity of these methods. Case studies were used to practically apply these calculation methods, and illustrate the significance of every step in the methodology developed. It was found that one is likely to obtain varying results. This could be mitigated by applying the methodology developed in this chapter.

Chapter 3 explored the opportunity to refine the prescribed methods from literature and investigate the potential for improvement. The prescribed methods (tier 3 specifically) were refined into a more complex, yet accurate approach by making use of the construction of mass balances. Case studies proved that by constructing an *advanced mass balance*, a much smaller error will be achieved, adding to the reliability of the final results.

Chapter 4 investigated and compared the variance, accuracy and complexity of the different methods (prescribed and developed). It was found that the application of the different quantification methods can lead to a variance of up to 33% on the calculated CO_2 emission result.

This translates to a variance of R185 million per year (R562 million ± R185 million) in carbon tax liability, just due to the use of different methods. The accuracy investigation found that a small error (<5%, suggested by literature) is only achievable when tier 3 is done thoroughly, as with mass balance 3. The complexity of each method was also investigated, and showed that one tends to obtain a much higher accuracy when slightly more complexity is added to the calculation method (e.g. MB2 to MB3).

Chapter 4 reviewed the results from Chapter 2 and Chapter 3 and compared the variance, accuracy and complexity of the different quantification methods. This was done by applying the different methods to 17 South African FeCr producing furnaces. The potential CT liability (monetary value) for the entire FeCr industry in SA has been estimated throughout the document in various ways. Table 5-1 gives a summary of the different cases, which will be discussed on the following page.

Table 5-1: FeCr industry carbon tax liability summary

Description	Sample size	Quantified carbon tax liability	Uncertainty associated with carbon tax liability	Maximum potential carbon tax liability for entire SA FeCr industry
1. Total CT liability based on literature	Total SA FeCr industry	Based on literature; Assumption: since FeCr production increased with ±30% over the last x year, the corresponding emissions also increased with that amount. ∴ Estimated CT liability = **R562 million**	Based on literature (Table); Maximum potential uncertainty according to IPCC = 50% ∴ Hence, estimated uncertainty = 50% of R562 = **R281 million**	R562 million ± R281 million ∴ Maximum potential = **R843 million**
2. Total CT liability based on literature and calculated variance (due to different quantification methods)	Total SA FeCr industry	Based on literature; Assumption: Since FeCr production increased with ±30% over the last x year, the corresponding emissions also increased with that amount. ∴ Estimated CT liability = **R562 million**	Average variance of all furnaces investigated: 13% - 33% variance (just due to the use of different methods) ∴ **R75 million - R185 million variance**	R562 million ± R185 million ∴ Maximum potential = **R747 million**
3. Total CT liability of 15 FeCr furnaces (based on Tier 1 method)	15 SA FeCr furnaces (±50% of total SA FeCr industry)	Sum of CO_2 emissions of all 15 FeCr furnaces for one year by using **Tier 1** method ∴ Estimated CT liability = **R258 million**	Average error of all furnaces investigated: T1: 37.5% of R258m ∴ **R97 million error**	R258 million ± R97 million ∴ Maximum potential = **R355 million** This value is for 15 furnaces only (±50% of total industry) ∴ Maximum potential for total FeCr industry **= R670 million**
4. Total CT liability of 15 FeCr furnaces (based on MB3 method)	15 SA FeCr furnaces (±50% of total SA FeCr industry)	Sum of CO_2 emissions of all 15 FeCr furnaces for one year by using **MB3** method ∴ Estimated CT liability = **R219 million**	Average error of all furnaces investigated: MB3: 2.4% of R219m ∴ **R5 million error**	R219 million ± R5 million ∴ Maximum potential = **R224 million** This value is for 15 furnaces only (±50% of total industry) ∴ Maximum potential for total FeCr industry **= R448 million**

The first row in Table 5-1, refers to the total CT liability based on literature, as calculated in Chapter 1 (page 3), and again in Chapter 4 (page 91). An estimated base CT liability of R562 million per annum was quantified, together with a 50% possible error (according to literature), resulting in a potential maximum amount of R843 million.

The next quantification used the same base liability (R562 million) as the previous, but with the variance calculated in Chapter 4 (Section 4.2). The uncertainty due to the use of different methods (variance) is estimated as a maximum of 33%, translating to a final CT liability of R747 million (maximum potential).

15 Furnaces were used to quantify the CO_2 emissions where all six methods were used. However, only the two extremes were showcased in the table (discussed in Section 4.3.3). Tier 1 and MB3 gave results of R355 million and R224 million, respectively. This is, however, for 15 furnaces only. It was assumed that these 15 furnaces represent ±50% of the FeCr industry in SA. These values were therefore normalised to quantify R670 million and R448 million, respectively. These four different quantifications are illustrated in Figure 5-1.

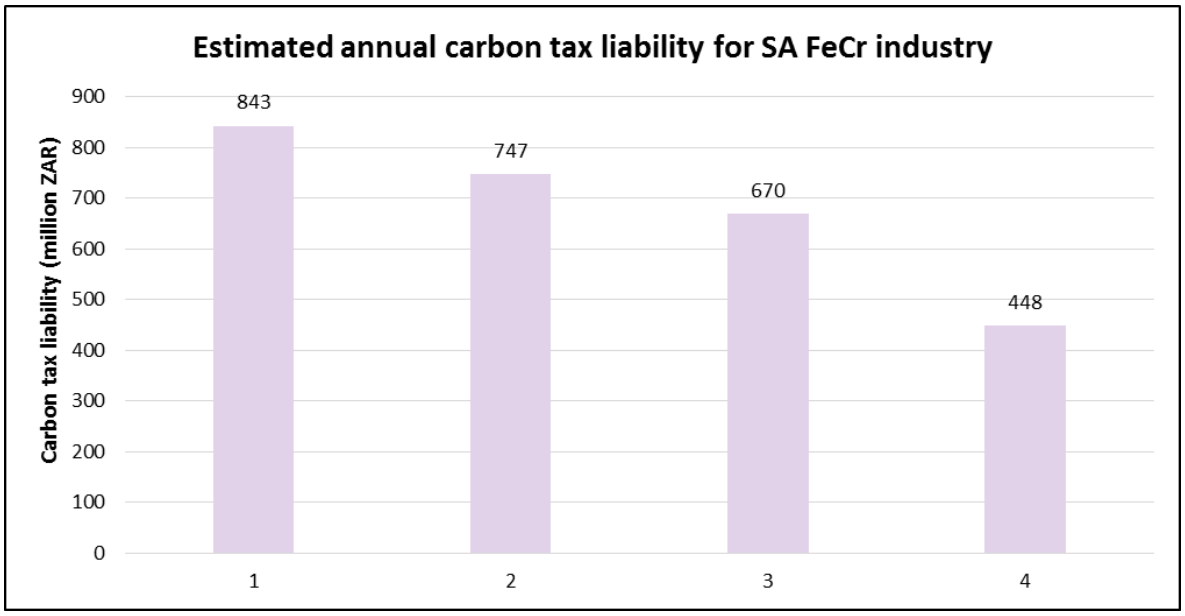


Figure 5-1: Estimated annual carbon tax liability for SA FeCr industry (based on Table 5-1)

Figure 5-1 shows how the initial estimation of the potential CT liability (monetary value) for the entire FeCr industry in SA has decreased throughout the course of this study. From a maximum potential annual value of R843 million (purely based on literature assumptions) to a value of R448 million (based on the use of MB3). This translates to a 47% decrease in CT liability.

5.2. Novel contributions

The main objective of this thesis was to critically analyse the CO_2 emission quantification methods used in the ferrochrome industry. The study undertook to provide several novel contributions to the field of emission quantification for the ferrochrome industry. These contributions were grouped into three categories (critical assessments, development of practical methods, and the quantification of implications for the South African FeCr industry), and were listed initially in Chapter 1. The following parts will provide detailed discussions and prove how these novel contributions were achieved.

5.2.1 Critical assessments

Bringing together available, but unrelated, literature and linking it to operational reality:

Assessment of the legal landscape, national and international resources available to the FeCr industry to highlight the lack of practical applications and examples.

At the beginning of this study, relevant background information on FeCr furnaces and the associated emissions was researched by means of the legal landscape, together with other relevant national and international references. Some uncertainties were identified in the form of research questions, which led to an in-depth critical literature review. 104 References were gathered and evaluated thoroughly to gain a basic knowledge and understanding of carbon tax, the ferroalloy industry and related GHG emissions (specifically in the FeCr industry). These references were categorised according to their focus of study and then scrutinised according to the research questions. This critical assessment led to the identification of certain gaps in literature and formulated the three focus areas of this study. [Section 1.3]

Critical assessment to establish a link between the prescribed legal processes and what is available from real-world operational systems.

The study critically assessed the prescribed legal processes on how to estimate the CO_2 emissions (and eventually the carbon tax liability) from a general FeCr furnace. The practical and operational workings of a typical FeCr furnace were also researched. These assessments established a link between what is required by carbon tax, as opposed to what is practically available from site. These results were combined in a unique way to estimate the emissions in the most accurate way possible. [Section 2.2.2; Section 2.2.4]

Critical assessment to highlight several practical constraints associated with the prescribed methods.

The practical application of the prescribed methods were evaluated based on real-world applications. This unique critical assessment led to the emphasising of certain constraints that could possibly arise during the implementation of these methods. These constraints were evaluated and shown to have a significant influence of the final results. [Section 2.3]

Critical assessment of coal composition analyses to determine the feasibility of practically determining the elemental composition of the reductant, based on operational measurements.

The chemical compositions of reductants were researched. A comprehensive study of reductant, the different types of analyses (proximate, ultimate and ash analyses) and the final elemental composition was conducted. This critical assessment lead to a unique way to establish the possible final elemental composition of reductant. [Section 3.2.2]

Critical assessment of available furnace characteristics from the iron- and steel industry for an application to quantify FeCr slag mass.

Research was done in terms of furnace characteristics from study fields other than the FeCr industry, i.e. the iron- and steel industry. This industry established that some compounds do not react chemically within the furnace. This statement led to the assumption that the FeCr slag mass could be estimated based on these non-reactive compounds. This introduced a unique way to estimate the mass of the slag for the FeCr industry. [Section 3.2.4]

5.2.2 Development of practical methods

The lack of clear guidance and detailed examples, together with multiple variances and possible errors, presents a challenge for objective assessment and evaluation of risks:

Development of a practical and systematic method to list assumptions, collect data, evaluate quality and apply the prescribed methods:†*

The prescribed methods simply provide the formulas to calculate the CO_2 emissions. However, Chapter 1 highlighted the lack of practical applications and examples in this area. A new practical method was therefore developed in order to do sufficient groundwork and understand the system being evaluated, which could possibly lead to better informed and more accurate estimations. [Section 2.3]

† *The author developed a similar approach on 12L work, published in SAJIE (2017). Appendix F.1* [152].

Development of a practical method to link compositional analyses to mass measurements.*

In order to perform an elemental mass balance, the mass of each stream must be assigned to a corresponding composition. It is found that there are not necessarily compositional analyses done on a daily basis, even though the specific material is consumed by the furnace every day. Another constraint is the uncertainty of when or where the analyses were done. If the raw material samples were analysed upon arrival/delivery, the material could have been stored in silos or stockpiles for an undefined period, creating a buffer capacity between the time of analysis and the time of batching to the furnace. A new approach was therefore developed to address these constraints and objectively link available compositional analyses to mass measurements. This method plays a critical role in the improved accuracy of mass balance results. [Section 3.3.3]

Development of a practical method to perform mass balances systematically from general to specific data.*

One of the prescribed CO_2 calculation methods is based on a mass balance approach. This is, however, given by a simple formula without any detail discussion or instructions/groundwork. A unique, practical method for constructing the mass balances was therefore developed. It uses six simple steps that are repeated for a literature-based mass balance (general), a measurement-based mass balance, and a detailed mass balance (specific data). This method was developed to obtain better and more accurate results. [Section 3.3.4; 3.3.5 - 3.3.7]

**The first three novel contributions of the 'Development of practical methods' are supported by the peer reviewed paper (conference proceedings, SAIIE 2018)* [153]*. This paper can be seen in Appendix F.2.*

Development of practical method to quantify and compare the accuracy and complexity associated with FeCr carbon tax calculations.

This study focused on six different methods to calculate the CO_2 emissions from a FeCr furnace. Some of the methods have higher accuracy than others, while some of them require more work and effort to complete. It was necessary to objectively compare these methods to one another. A unique method was therefore developed to practically quantify the accuracy and complexity of the different methods. [Section 4.3.34.3]

5.2.3 Quantification of implications for SA FeCr industry

This thesis verified and validated its various methodologies using 17 case studies from the South African FeCr industry. These case studies represent ±50% of SA's FeCr fleet and is therefore a significant indicator of local industry challenges and risks:

Quantification of the impact of operational errors

The prescribed methods provide formulas to be completed in order to calculate the CO_2 emissions from a FeCr furnace. These prescribed methods were applied and tested with induced operational errors that may commonly occur. The average effect that these potential errors can have on the final CO_2 emission results are quantified as: 18.8% (effect of incorrect information and layouts of the plant), 11.2% (effect of using the incorrect emission factors), and 8.9% (effect of poor data quality). [Section 2.4]

Quantification of the accuracy change in mass balances

The refinement of tier 3 (mass balance approach) led to the development of three mass balances: a mass balance based on literature values and assumptions (MB1), a mass balance based on measured values (MB2) and an advanced, detailed mass balance (MB3). The associated errors of these three phases of mass balances were quantified, and on average gave the following results: 17.0% error (MB1), 13.3% error (MB2) and 2.4% error (MB3). [Section 3.4]

Quantification of the variances between the different methods

The CO_2 emission results from the six quantification methods vary significantly from one another. This variance was therefore quantified for 15 different furnaces. This significant variance was quantified by two different approaches, including the range method (difference between the minimum value and the maximum value) and the standard deviation (concentration of the data around the mean of the dataset), giving a 13% difference based on the standard deviations, and a 33% difference according to the range method. [Section 4.2]

Quantification of the complexities of the different methods

Some of the CO_2 quantification methods require more complex applications than others. Where tier 1 only requires the amount of FeCr produced and a generic production emission factor, some of the mass balances would require many complex calculations, assumptions and interpretations. To compare the different quantification methods objectively in terms of the complexity, three factors were considered: the number of references, the number of variables and the number of calculations. These three complexity factors were summed together to obtain a complexity value for each method: 4 (T1), 23 (T2), 24 (T3), 76 (MB1), 82 (MB2), and 84 (MB3). [Section 4.3.2]

Quantification of the estimated industry exposure (SA FeCr carbon tax liability)

Different methods and newly-developed approaches were used to evaluate CO_2 emissions from FeCr furnaces. Even though only 17 (of which 15 are AC) SA furnaces were investigated in terms

of the CO_2 emissions, the results were extrapolated to estimate the total for SA. This was done to estimate the final carbon tax liability of the FeCr industry in SA. The final quantified value was initially estimated as R562 million ± R281 million per annum, but through the course of the study, decreased to a value of R438 million ± R10 million (see Table 5-1). [Thesis]

5.3. Recommendations for future work

Recommendations for further studies are listed below. Additional research in these areas has the potential to further improve the results presented in this study:

Different furnace technologies may require refined methods of CO_2 quantification:

Problem: The variances of the DC furnaces highlighted in Chapter 4 (see F3 and F4 in Figure 4-3) were significantly higher than those of the AC furnaces.

Recommendation: Do more extended literature research in terms of the different furnace technologies (AC vs. DC; open vs. closed furnaces; etc.). The fundamental difference in furnace characteristics could indicate where the focus must be in terms of refining the CO_2 quantification methods.

Sensitivity of results due to variance in selected parameters:

Problem: The influence of different parameters (e.g. carbon content of certain streams, moisture, etc.) of a FeCr furnace regarding the CO_2 emissions is unknown. There is thus no indication of where to focus when trying to monitor/control the CO_2 emissions.

Recommendation: Conduct a sensitivity analysis to indicate which parameters have the largest influence on the calculated CO_2 result. The measurement of this identified parameter(s) can then be given a higher priority when improving the quality of the measurements.

Ash analysis uncertainty:

Problem: Ash analyses are done in the presence of other elements, causing the reported analysis to be an imperfect representation of the raw coal ash. This is usually done to indicate the ratio between certain significant

elements. The ash component of all reductants was therefore assumed as "trace elements".

Recommendation: Do more research in terms of the elemental composition of raw coal ash. The total elemental composition (TEC) of the reductants can then be adjusted to include the elements from ash, and therefore obtain more accurate results.

Develop an improved emission factor or equation:

Problem: It was found that, with more complexity, one is likely to achieve more accurate results (e.g. MB3). However, having too complex methods can lead to time- and other constraints in industry.

Recommendation: The results from MB3 can be used to develop a new emission factor or equation (as in T1), where the complexity of MB3 will be combined with the simplicity of a T1 calculation. Such an equation would explore different types of models (linear vs. polynomial), and parameters featured in the equation (FeCr production; reductant mass and composition, etc.).

Additional applications of the advanced mass balance developed:

Problem: The aim of this study was focused on the quantification of CO_2 emissions, and ultimately carbon tax. However, the results may have other, unrelated applications.

Recommendation: An additional application of the furnace model/balance would enable improved operational control of the furnace, and allow informed decision-making and predictions. The model could be adjusted slightly to predict the outcome of any changes made, e.g.: How would the composition of the product vary if the raw material mix is changed? How much more product will be produced if the raw materials are of better quality? How will the energy consumption of the furnace be influenced by using a different raw-material mix? How can the off-gas emissions be limited/decreased?

This model can later be automated to run various scenarios before any operational decisions are made. The chemical reactions can also be considered to estimate the energy consumption of the furnace, based on the heat of reaction (ΔH) of each chemical reaction.

Testing/refining of slag mass calculation:

Problem: The amount of Al_2O_3 present in the furnace is used to determine the slag mass in MB3 (Equation 3-22), since it doesn't react chemically. The compounds MgO and CaO also doesn't react, but is not considered in the calculations for slag mass.

Recommendation: The slag mass calculated by MB3 can be verified or refined by making use of MgO and CaO contents as well.

5.4. Final conclusion

This thesis evaluated the CO_2 emission quantification methods of the FeCr industry. The prescribed calculation methods (tier 1, 2 and 3) were assessed in terms of their practical applicability, since no sufficient practical examples of application could be found in literature. Case studies illustrated that, without the methodology developed, one is likely to obtain less accurate results (possible errors of 8.9% - 18.8%) when performing the prescribed methods.

It was found that the prescribed methods used to quantify CO_2 emissions are not necessarily accurate, and may also vary from one another. The construction of mass balances (MBs) was used to explore the idea of refining the prescribed methods. Case studies proved that by constructing a detailed MB, a smaller error can be achieved (2.4%), adding to the reliability of the results.

The application of different quantification methods gave a variance of 13-33% on the calculated CO_2 emission result. Hereafter, the accuracy of the different methods were compared. According to literature, tier 1 is less accurate (25%-50% error) than tier 3 (<5% error). However, if this is implemented practically, it is evident that this small error (<5%) is only achievable when tier 3 is done thoroughly, as with the detailed mass balance. The complexity of the different methods increased significantly between the prescribed methods and the refined mass balances. It was found, however, that with a little extra "complexity" a much higher accuracy can be accomplished. Based on the method developed throughout this study, and

A significant contribution of the approach is realised by improved CT liability estimation. The monetary value for the entire FeCr industry in SA has decreased throughout the course of this study. From an initial estimation of R562 million per annum with a 50% uncertainty (purely based on literature assumptions) to a value of R448 million with a 2.4% uncertainty (based on the use of methods developed within this study). The developed approach is therefore confirmed to make a critical contribution to the emission quantification for FeCr furnaces.

Bibliography

[1] J. Roos and A. Hearn, "Optimising the effective use of energy in the ferroalloy industry through innovative technology," in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town, 2004.

[2] Y. Xiao, Y. Yang and L. Holappa, "Tracking chromium behaviour in submerged arc furnace for ferrochrome production," *2006 TMS Fall Extraction & Processing Meeting: Sohn Int'l Symposium*, pp. 583-594, 2006.

[3] M. Riekkola-Vanhanen, "Finnish expert report on best available techniques in ferrochromium production," Finnish environment insitute, Helsinki, 1999.

[4] Y. Otani and K. Ichikawa, "Manufacture and Use of Prereduced Chromium-ore," in *Infacon I - Proceedings of 1st International Ferroalloys Congress*, Johannesburg, 1974.

[5] L. Holappa, "Toward sustainability in ferroalloys," in *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki, 2010.

[6] X. Pan, "Effect of South African reductants on ferrochrome production," in *Infacon XIV - Proceedings of Fourteenth International Ferroalloys Congress*, Kiev, 2015.

[7] K. Bergman and B. Kjellberg, "DC Arc Furnace Technology Applied to Smelting Applications," Helsinki, 1997.

[8] X. Pan, "Learning and teaching using process modelling and simulation," in *International Conference on Mining, Minerals and Metallurgical Engineering*, Harare, 2015.

[9] Ideas 1st Research, "Ferrochrome," Ideas 1st Research, Mumbai, 2010.

[10] J. Hattingh and J. Friend, "Environmental and economic implications of slag disposal practices by the ferrochromium industry: A case study," *South African water research commission*, vol. 29, 2003.

[11] S. Du Preez, "Cr(VI) generation during flaring of off-gas from closed ferrochromium submerged arc furnaces," North West University, Potchefstroom, 2014.

[12] Anon, "Reductant characteisation in ferroalloys," University of the Witwatersrand, Johannesburg, 2004.

[13] G. Kapure, C. Kari, S. M. Rao and K. S. Raju, "Use of chemical energy in submerged arc furnace to produce ferrochrome: prospects and limitations," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[14] P. Niemelä, H. Krogerus and P. Oikarinen, "Formation, characteristics and utilisation of cogas formed in ferrochromium smelting," in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town, 2004.

[15] J. Beukes, N. Dawson and P. Van Zyl, "Theoretical and practical aspects of Cr(VI) in the South African ferrochrome industry," in *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki, 2010.

[16] T. Lindstad, S. Olsen, G. Tranell, T. Færden and J. Lubetsky, "GHG emissions from ferro-alloy production," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2006.

[17] Norway, "National Inventory Report 2008," The Norwegian Pollution Control Authority (SFT);, Oslo, 2008.

[18] J. Daavittila, M. Honkaniemi and P. Jokinen, "The transformation of ferrochromium smelting technologies during the last decades," *The Journal of The South African Institute of Mining and Metallurgy*, no. 9, pp. 541-549, 2004.

[19] Department of Environmental Affairs, "Declaration of greenhouse gases as priority air pollutants," *Government gazette*, vol. 710, no. 40996, pp. 65-69, 2017.

[20] A. Gous, "A practical approach to quantify carbon tax in South Africa," North-West University, Potchefstroom, 2017.

[21] "President Jacob Zuma to attend high level segment of Conference of the Parties (COP-15) in Copenhagen," South African Government, 8 December 2009. [Online]. Available: http://www.gov.za/president-jacob-zuma-attend-high-level-segment-conference-parties-cop-15-copenhagen. [Accessed 21 January 2017].

[22] J. Booysen, "Strategy to identify and prioritise risks for carbon tax in South Africa," *SAJIE*, 2017.

[23] M. Gigaba, "Budget Speech," National Treasury, Pretoria, 2018.

[24] T. Mboweni, "Medium Term Budget Policy Statement 2018," National Treasury, Pretoria, 2018.

[25] National Treasury, "Draft Carbon Tax Bill," vol. 2, no. 1-65, 2017.

[26] W. Biermann, R. Cromarty and N. Dawson, "Economic modelling of a ferrochrome," *The Journal of The Southern African Institute of Mining and Metallurgy*, vol. 112, pp. 301-308, 2012.

[27] T. Letete, M. Guma and A. Marquard, “Information on climate change in South Africa: greenhouse gas emissions and mitigation options,” Energy Research Centre , Cape Town, 2015.

[28] K. Ratshomo, “South Africa's ferroalloys production trends (REPORT R92/2012),” Department of Mineral Resources, Pretoria, 2012.

[29] Department of Mineral Resources, “MB Bulletin,” *Directorate: Mineral economics,* vol. 29, no. 2, 2016.

[30] Y. Lozynskyy, M. Neelis, P. Blinde, Y. Lewis, B. Cohen, A. Van der Merwe and I. Patel, “Emissions intensity benchmarks for the South African carbon tax - Technical support study,” ECOFYS, Utrecht, 2014.

[31] National Treasury, “Draft regulations for carbon offsets,” 2016.

[32] Department of Environmental Affairs, “National greenhouse gas emission reporting regulations,” vol. 622, no. 40762, pp. 4-24, 2017.

[33] National Treasury, “Media statement - Release of Carbon Tax Bill for introduction in parliament and public comment,” South Africa, 2017.

[34] Department of Environmental Affairs, “Technical guidelines for monitoring, reporting and verification of greenhouse gas emissions by industry,” Government printer, Pretoria, South Africa, 2017.

[35] S. H. Eggleston, L. Buendia, K. Miwa, T. Ngara and K. Tanabe, “IPCC guidelines for national greenhouse gas inventories,” IGES, Japan, 2006.

[36] J. McMurry, Organic chemistry, 7th ed., Thomson Brooks/Cole, 2008.

[37] S. Olsen, B. Monsen and T. Lindstad, “CO2 emissions from the production of manganese and chromium alloys in Norway,” in *ISS, Electric furnace conference proceedings*, Trondheim, 1998.

[38] T. Lindstad, S. Olsen, G. Tranell, T. Faerden and J. Lubetsky, “Greenhouse gas emissions from ferroalloy production,” in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[39] J. Basson, T. Curr and W. Gericke, “South Africa's ferroalloys industry - present status and future outlook,” 2006.

[40] M. Visser, “An overview of the history and current operational facilities of Samancor Chrome,” *Southern African Pyrometallurgy*, pp. 285-296, 2006.

[41] Y. Yang, Y. Xiao and M. Reuter, "Analysis of transport phenomena in submerged arc furnace for ferrochrome production," in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town, 2004.

[42] S. Ranganathan, "Optimisation of specific power consumption in the production of ferroalloys through rationalisation of charge distribution," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[43] J. Beukes, P. Van Zyl and M. Ras, "Treatment of Cr(VI)-containing wastes in the South African ferrochrome industry - a review of currently applied methods," *The Journal of The Southern African Institute of Mining and Metallurgy*, vol. 112, pp. 347-352, 2012.

[44] W. Gericke, "Environmental aspects of ferrochrome production," in *Infacon VII - Proceedings of 7th International Ferroalloys Congress*, Trondheim, 1995.

[45] R. Jones, T. Reynolds and T. Curr, "Some myths about DC arc furnaces," in *Southern African Pyrometallurgy*, Johannesburg, 2011.

[46] G. Denton, J. Bennie and A. De Jong, "An improved DC arc process for chromite smelting," in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town, 2004.

[47] H. Weitz, "Evaluation of the furnace method for the production of low carbon ferrochrome," University of Pretoria, Pretoria, 2015.

[48] L. Holappa and Y. Xiao, "Slags in ferroalloys production - review of present knowledge," *The Journal of The South African Institute of Mining and Metallurgy*, pp. 429-438, 2004.

[49] J. Kunze and R. Degel, "New trends in submerged arc furnace technology," in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town, 2004.

[50] M. M. Gasik, Handbook of ferroalloys: Theory and technology, Espoo: Elsevier, 2013.

[51] P. Bhonde, A. Ghodganonkar and R. Angal, "Various techniques to produce low carbon ferrochrome," in *Infacon XI - Proceedings of 10th International Ferroalloys Congress*, New Delhi, 2007.

[52] Y. N. Chesnokov, V. Lisienko and A. Lapteva, "Evaluating the carbon footprint from the production of steel in an electric-arc furnace," *Metallurgist*, vol. 57, no. 10, pp. 774-778, 2014.

[53] L. Els, F. Fereday and O. Corster, "Major ferroalloy producer improves furnace fume control system by installing baghouse with membrane filter bags," in *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki, 2010.

[54] U. S. Environmental Protection Agency, "Ferroalloy production," EPA, 2011.

[55] M. Erwee, "Andalusite as slag conditioner in ferrochrome production: A case study in techo-ecnomic modelling," in *Infacon XIII - Proceedings of 13th International Ferroalloys Congress*, Almaty, 2013.

[56] T. Faerden, "Environmental standards and the ferroalloy industry," in *Infacon VII - Proceedings of 7th International Ferroalloys Congress*, Trondheim, 1995.

[57] M. Farjadi and J. Azari, "Effect of chrome ore quality on ferrochrome production efficiency," in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town.

[58] S. Gradahl, S. Johansen, B. Ravary, B. Andresen and H. Tveit, "Reduction of emissions from ferroalloy furnaces," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[59] L. Hunsbedt, P. Cowx, R. Flatabo, K.-E. Johansen and J. Bustnes, "Environmental challenges for Norwegian Mn-industry," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[60] A. Jones, "The market & cost environments for bulk ferroalloys," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[61] A. Jones, "Carbon reductants for the production of chrome and manganese alloys," in *Infacon XII - Proceedings of the 12th International Ferroalloys Congress*, Helsinki, 2010.

[62] ENRC: Marketing, "Issues facing the ferrochrome industry," ENRC, Hong Kong, 2013.

[63] E.-P. Heikkinen and T. Fabritius, "Modelling of the refining processes in the production of ferrochrome and stainless steel," University of Oulu, Oulu, 2012.

[64] S. A. C. Hockaday and K. Bisaka, "Some aspects of the production of ferrochrome alloys in pilot DC arc furnaces at Mintek," in *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki, 2010.

[65] ICDA, "Discover Chromium - Ore Processing," International Chromium Development Association, 2011.

[66] Industrial Energy Management Training Course, "Energy Monitoring, Targeting & Reporting," Industrial Energy Management Training Course, 2002.

[67] R. Koekemoer, O. Vorster, F. Fereday, C. Els, L. Els and C. Coetzee, "Air pollution control system upgrade at Tubatse Ferrochrome," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[68] D. W. Ksinsik, “Reflections on the future and on the role of the ferroalloys industry in the development of North America,” in *Infacon VII - Proceedings of 7th International Ferroalloys Congress*, Trondheim, Norway, 1995.

[69] A. Lomo, Pollution problems with electric reduction furnaces in the ferro-alloy industry, Union Carbide Corporation, USA.

[70] G. Makhoba and R. Eric, “Reductant characterisation and selection for ferrochromium production,” in *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki, 2010.

[71] Merafe resources, “Annual integrated report 2015,” Merafe resources, Johannesburg, 2015.

[72] Metallurial industry, “Ferroalloy production - Emission factors,” 1989.

[73] K. Mills, “The estimation of slag properties,” Southern African Pyrometallurgy, London, 2011.

[74] B. Monsen, T. Lindstad and J. Tuset, “CO2 emissions from the production of ferrosilicon and silicon metal in Norway,” in *Electric furnace proceedings*, Trondheim, 1998.

[75] M. Mosiane, “The impact of chrome ore exportson the local ferrochrome industry,” Department of Minerals and energy, Pretoria, 2007.

[76] NAPCA, “Air pollutant emission factors,” National air pollution control administration, Washington D.C., 1970.

[77] M. A. Nkohla, “Characterization of ferrochrome smelter slag and its implications in metal accounting,” Cape Peninsula University of Technology, Cape Town, 2006.

[78] National Pollutant Inventory, “Emission estimation technique manual for ferroalloy production,” Environment Australia, Canberra, 1999.

[79] K. Penttilä, “ChemSheet Modelling,” VTT technical research centre if Finland Ltd, Oulu, 2016.

[80] R. Person, “Pollution abatement of ferro-alloy furnaces in the United States,” in *Orinoco Chemical Products*, 1983.

[81] E. Pezennec, “Key results of the initial environmental risk assessment for chromium III compounds and chromium metal,” in *Infacon XI - Proceedings of 10th International Ferroalloys Congress*, New Delhi, 2007.

[82] Sri Sai Manasa Nature Tech Pvt. Ltd, “Environmental impact assessment for expansion of ferro alloys unit production,” Andhra Pradesh, India, 2017.

[83] E. Scheepers, Y. Yongxiang, A. T. Adema, R. Boom and M. A. Reuter, "Process modeling and optimization of a submerged arc furnace for phosphorus production," *Metallurgical and materials transactions,* vol. 41B, pp. 990-1005, 2010.

[84] R. Garcia-Segura, J. V. Castillo, F. Martell-Chavez, O. Longoria-Gandara and J. O. Aguilar, "Electric Arc Furnace Modeling with Artificial Neural Networks and Arc Length with Variable Voltage Gradient," *Energies,* vol. 10, no. 1424, pp. 1-11, 2017.

[85] R. K. Taggart, J. C. Hower, G. S. Dwyer and H. Hsu-Kim, "Trends in the Rare Earth Element Content of U.S.-Based Coal Combustion Fly Ashes," *Environmental Science & Technology,* vol. 50, pp. 5919-5926, 2016.

[86] U.S. Environmental Protection Agency, "Background report - Ferroalloy production," U.S. Environmental Protection Agency, Research Triangle Park (NC), 1992.

[87] A. K. Vaish, "Pollution Control in Ferro-Alloys Production," National Metallurgical Laboratory, Jamshedpur, 1992.

[88] Visagie, "Eskom and the ferrochrome industry," 2006.

[89] Xstrata, "Maximising South Africa's chrome ore endowment to create jobs and drive sustainable growth," Xstrata, Pretoria, 2011.

[90] O. Zayakin, V. Zhuchkov and B. Afanasiev, "Study of Carbothermic Reduction Processes in Manufacture of High-carbon Ferrochrome," Kiev, 2015.

[91] R. Goel, "Smelting Technologies for Ferrochromium Production - Recent Trends," in *National Metallurgical Laboratory*, Jamshedpur, 1997.

[92] C. Harman and N. Rama Rao, "Use of sintered pellets in production of high carbon ferro-chrome," in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[93] ADEME, "Understanding the issues around quantifying GHG emissions in the financial sector," ADEME, Paris, 2016.

[94] APTA, "Recommended practice for qualifying greenhouse gas emissions from transit," APTA Climate Change Standards Working Group, 2009.

[95] CAPCOA, "Quantifying greenhouse gas mitigation measures," California Air Pollution Control Officers Association, 2010.

[96] M. Chen and O. Johnson, "Quantifying and managing supply chain creenhouse gas emissions," Stanford global supply chain management forum, 2011.

[97] Defra, "Guidance on how to measure and report your greenhouse gas emissions," Department of energy & climate change, London, 2009.

[98] C. Frey, "Quantification of uncertainty in emission factors and inventories," in *Department of Civil, Construction, and Environmental Engineering*, Raleigh (NC), 2007.

[99] T. Hiraishi, B. Nyenzi and R. Odingo, "Quantifying uncertainties in practice," IPCC Good Practice Guidance and Uncertainty Management 6.4 in National Greenhouse Gas Inventories.

[100] IPIECA, "Petroleum industry guidelines for reporting greenhouse gas emissions," 2011.

[101] R. Kühn, H. G. Geck and K. Schwerdtfeger, "Continuous off-gas measurement and energy balance in electric arc steelmaking," *ISIJ International*, vol. 45, no. 11, pp. 1587-1596, 2005.

[102] E. Milne, "Methods for the quantification of GHG emissions at the landscape level for developing countries in smallholder contexts," *Environmental Research Letters*, vol. 8, no. 015019, pp. 1-9, 2013.

[103] V. Sonntag-O'Brien, "Strategic framework for quantifying, monitoring, evaluating and reporting local greenhouse gas emissions reductions," in *Workshop on Best Practices in Policies and Measures*, Copenhagen, 2000.

[104] A. Young, "GHG plan level quantification guidance," 2010.

[105] S. Banerjee, "The world of chromite ore," Tata Steel Ltd, Chromium 2006, Cape Town, 2006.

[106] B. P. Bhardwaj, The complete book on ferroalloys, New Delhi: NIIR Project Consultancy Services (NPCS), 2014.

[107] Environmental Protection Act, "Ontario Regulation 452/009 - Greenhouse gas emissions reporting," Environmental Protection Act, Toronto, 2016.

[108] V. Vellinga, H. Blonk, M. Marinussen, W. Van Zeist, I. De Boer and D. Starmans, "Methodology used in FeedPrint: a tool quantifying greenhouse gas emissions of feed production and utilization," Wageningen UR Livestock Research, Wageningen, 2013.

[109] The Norwegian Emission Inventory 2016, "Documentation of methodologies for estimating emissions of greenhouse gases and long-range transboundary air pollutants," Statistics Norway, Oslo, 2016.

[110] Partnership for Market Readiness, "Emissions quantification," Carbon Finance, Beijing, 2013.

[111] T. Epstein, “Ferroalloy Furnace Emission Factor Development,” U. S. Environmental Protection Agency, Washington DC, 1981.

[112] Fredriksen and Nestas;, “Pollution Problems - Electric Furnace Ferroalloy Production,” United Nations Economic Commission for Europe, 1968.

[113] S. Gronberg, “Ferroalloy Industry Particulate Emissions,” U. S. Environmental Protection Agency, Cincinnati (OH), 1986.

[114] J. McLaughlan, “Challenges facing the South African ferrochrome industry,” Chromium 2006, Cape Town, 2006.

[115] J. Rudolph, “Ferroalloy Process Emissions Measurement,” U. S. Environmental Protection Agency, Washington DC, 1979.

[116] Iron and Steel Institute, *Journal of the Iron and Steel Institute,* vol. 93, no. 1, 2012.

[117] G. Westbrook and D. Dougherty, “Environmental Impact of Ferroalloy Production Interim Report: Assessment of Current Data,” Research Triangle Institute, Research Triangle, 1978.

[118] Umwelt Bundesamt, “CO2 Emission Factors for Fossil Fuels - Climate change 28/2016,” German Environment Agency, Germany, 2016.

[119] U. S. Environmental Protection Agency, “Emission Factors for Greenhouse Gas Inventories,” 2018. [Online]. Available: https://www.epa.gov/sites/production/files/2018-03/documents/emission-factors_mar_2018_0.pdf. [Accessed 10 July 2018].

[120] D. Sager, D. Grant, R. Stadle and T. Schreiter, “Low cost ferroalloy extraction in DC-arc furnace at Middleburg Ferrochrome,” *The Journal of The Southern African Institute of Mining and Metallurgy,* vol. 110, pp. 717-724, 2010.

[121] B. Broekman and K. Ford, “The development and application of a HCFeMn furnace simulation model for Assmang Ltd.,” in *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town, 2004.

[122] C. Harman and N. Rama Rao, “Use of sintered pellets in production of high carbon ferrochrome,” in *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi, 2007.

[123] J. Van Doorn, P. Bruyn and P. Vermeij, “Combined combustion of biomass, municipal sewage sludge and coal in an atmospheric fluidized bed installation,” in *9th European bioenergy conference,* 1996.

[124] Y. Sun, . S. Sridhar, . S. Seetharaman, H. Wang, L. Liu, X. Wang and Z. Zhang, "A Fe-C-Ca big cycle in modern carbon-intensive industries: toward emission reduction and resource utilization," *Energy science and technology*, 2016.

[125] H. Van der Sloot and P. Cnubben, "Verkennende evaluatie kwaliteitsbeinvloeding poederkoolvliegas," ECN-report, 2000.

[126] C. Klein and A. Philpotts, Earth materials - Introduction to mineralogy and petrology, Cambridge: Cambridge University Press, 2017.

[127] M. O'Brien and W. Wood, The prehistory of Missouri, Columbia: University of Missouri Press, 1998.

[128] J. Götze and R. Möckel, Quartz: Deposits, mineralogy and analytics, Heidelberg: Springer, 2012.

[129] Lhoist North America, "Material Safety Data Sheet - Quicklime," Lhoist North America, 2012.

[130] F. R. Sprinzl, "Valorization of ferrochrome slag: Towards increasing the beneficial utilisation of ferrochrome slag in South Africa," Stellenbosch University, Stellenbosch, 2016.

[131] T. N. Herzog, F. J. Scheuren and W. E. Winkler, Data quality and record linkage techniques, Springer, 2007.

[132] W. Booysen, "Measurement and verification of industrial DSM projects," North-West University, Potchefstroom, 2014.

[133] J. Speight, "Handbook of coal analysis," John Wiley & Sons, Hoboken (NJ), 2005.

[134] South African National Standard, "SANS 17247:2006 Coal - ultimate analysis," SABS Standards division, Pretoria, 2006.

[135] Sanas, "Central coal laboratory - Test report," Sanas, Pretoria, 2017.

[136] H. Pinheiro, C. Pretorius and H. Boshoff, "Analyses of coal and product samples of South African collieries 1998-1999," SABS, Pretoria, 1999.

[137] D. W. Green and R. H. Perry, Perry's chemical engineers' handbook. 8th Ed., New York City (NY): McGraw-Hill, 2008.

[138] International Standard, "ISO 1213-2: Solid mineral fuels - Part 2: Terms relating to sampling, testing and analysis," ISO, Geneva, Switzerland, 2016.

[139] B. Agarwal, Basic statistics, New Delhi: New age international (P) Ltd., 2006.

[140] C. P. McKeague, Basic Mathematics, 7th Ed., Belmont (CA): Brooks/Cole Cengage learning, 2010.

[141] D. J. Rumsey, Statitics for dummies, 2nd Ed., Hoboken (NJ): John Wiley & Sons, 2016.

[142] Statistics How To, "Statistics How To," 2018. [Online]. Available: http://www.statisticshowto.com/probability-and-statistics/normal-distributions/#whatisND. [Accessed 13 August 2018].

[143] J. Devore and N. Farnum, Applied statistics for engineers and scientists. 2nd Edition., Belmont (CA): Brooks/Cole, Cengage Learning, 2005.

[144] H. Maltby, S. Kailasa and A. Ellinor, "Normal distribution," Brilliant.org, 2018. [Online]. Available: https://brilliant.org/wiki/normal-distribution/. [Accessed 13 August 2018].

[145] D. M. McEvoy, A guide to business statistics, Hoboken (NJ): John Wiley & Sons, 2018.

[146] R. M. Felder and R. W. Rousseau, Elementary principles of chemical processes, Hoboken (NJ): John Wiley & Sons, Inc., 2005.

[147] J. Ruuska, A. Sorsa, J. Lilja and K. Leiviskä, "Mass-balance based multivariable modelling of basic oxygen furnace used in steel industry," in *International Federation of Automatic Control, Elsevier Ltd.*, Oulu, 2017.

[148] A. Bhattacharya and S. Muthusamy, "Static heat energy balance mathematical model for an iron blast furnace," *International Journal of Mineral Processing and Extractive Metallurgy*, vol. 2, no. 5, pp. 57-67, 2017.

[149] G. Mandal, D. Sau and S. Das, "A steady state thermal and material balance model for an iron making blast furnace and its validation with operational data," *Indian Institute of Metals*, vol. 67, no. 2, pp. 209-221, 2014.

[150] A. A. Akbar, "Materials and energy balances - Charge calculations in pyrometallurgical processes," Department of Production Engineering and Metallurgy, University of Technology, Iraq, Bagdad.

[151] G. Kleinschmidt, R. Degel, M. Köneke and H. Oterdoom, "AC and DC smelter technology for ferrous metal production," in *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki, 2010.

[152] K. Campbell, W. Booysen and J. C. Vosloo, "Evaluating tht feasibility of the 12L tax incentive for energy-intensive industries," *South African Journal of Industrial Engineering (SAJIE)*, vol. 28, no. 3, pp. 15-28, 2017.

[153] K. Campbell, W. Booysen and M. Kleingeld, “Using data-driven analytics to develop a material banace over a ferrochrome furnace.,” in *Southern African Institute for Industrial Engineering* , Stellenbosch, 2018.

[154] F. Henglein, Chemical technology, Weinheim: Verlag chemie, 1969.

A. APPENDIX A: Critical study

PHASE 1:

Table A-1: Reference type distribution (Phase 1)

Type of reference	Percentage	Number
Journal article	17%	17
Conference paper	37%	38
Thesis / dissertation	5%	5
National official documentation	18%	19
Book	2%	2
Report	13%	13
Training course material	7%	7
Other	2%	2
Total	**100%**	**103**

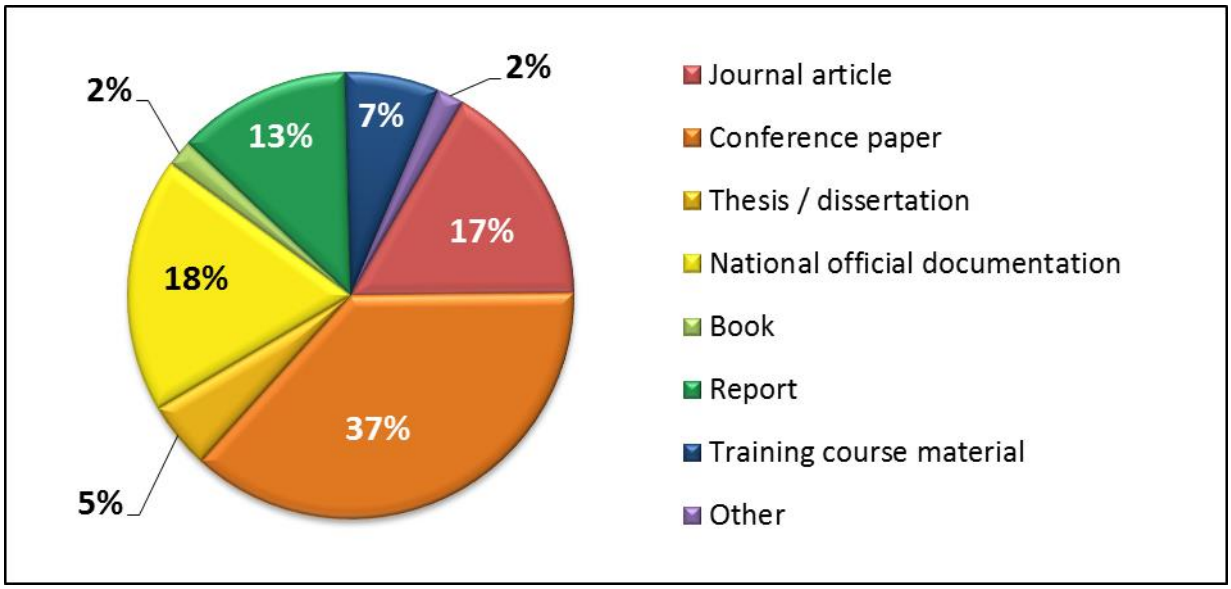


Figure A-1: Reference type distribution (Phase 1)

Table A-2: Phase 1 of critical literature review

Ref. nr.	Reference	Type of ref.	Year	Focus of reference study						Ref. nr. *(ref. list)*
				Energy	Production	Economics	Modelling	Environment	Quantifying emissions	
1	Anon (M)	T/D	2004		X		X			[12]
2	ADEME	N/OD	2016					X	X	[93]
3	APTA	N/OD	2009					X	X	[94]
4	Banerjee	R	2006		X	X				[105]
5	Basson	CP	2006			X	X			[39]
6	Bergman	CP	1997	X	X					[7]
7	Beukes	CP	2010	X	X	X				[15]
8	Beukes	JA	2012		X					[43]
9	Bhardwaj	B	2014	X	X					[106]
10	Bhonde	CP	1985		X					[51]
11	Biermann	JA	2012	X	X	X	X	X		[26]
12	Booysen	JA	2017					X	X	[22]
13	CAPCOA	N/OD	2010					X	X	[95]
14	Chen & Johnson	R	2011					X	X	[96]
15	Chesnokov	JA	2013					X	X	[52]
16	Daavittila	JA	2004	X	X	X		X		[18]
17	Defra	R	2009					X	X	[97]
18	Denton	CP	2004	X	X	X	X	X		[46]
19	Dept. of environmental affairs	N/OD	2017					X	X	[32]
20	Dept. of environmental affairs	R	2017					X	X	[34]
21	Du Preez	T/D	2014		X		X	X		[11]
22	Els	CP	2010				X	X		[53]
23	ENRC	CP	2013		X	X				[62]
24	Environmental protection act	R	2016					X	X	[107]
25	EPA	N/OD	2011		X			X	X	[54]
26	Epstein	R	1981				X	X		[111]
27	Erwee	CP	2013	X	X					[55]
28	Faerden	CP	1995	X				X		[56]
29	Farjadi & Azari	CP	2004	X	X	X				[57]
30	Fredriksen and Nestas	JA	1968					X		[112]
31	Frey	R	2007				X	X		[98]
32	Gasik	B	2013	X	X	X		X		[50]
33	Gericke	CP	1995		X	X		X		[44]
34	Gous	T/D	2017					X	X	[20]
35	Gradahl	CP	2007				X	X		[58]
36	Gronberg	JA	1981					X		[113]
37	Hattingh	JA	2003		X	X		X		[10]
38	Heikkinen	TCM	2012	X	X		X			[63]
39	Hockaday & Bisaka	CP	2010	X	X					[64]
40	Holappa	CP	2010	X	X	X		X	X	[5]
41	Holappa & Xiao	JA	2004		X		X			[48]
42	Hunsbedt	CP	2007					X		[59]
43	ICDA	N/OD	2011	X	X					[65]
44	Industrial EnM training	TCM	2002	X			X	X		[66]
45	IPCC	N/OD	2006					X	X	[35]
46	IPCC	R	2006					X	X	[99]
47	IPIECA	R	2011					X	X	[100]

48	Jones	CP	2007		X	X				[60]
49	Jones	CP	2010			X				[61]
50	Jones	JA	2011		X		X			[45]
51	Kapure	CP	2007	X	X					[13]
52	Koekemoer	CP	2007				X	X	X	[67]
53	Ksinksik	CP	1995		X	X				[68]
54	Kunze	CP	2004	X	X					[49]
55	Lindstad	CP	2006					X	X	[16]
56	Lindstad	CP	2010					X	X	[38]
57	Lomo	CP	n.d.					X		[69]
58	Lozynskyy et al.	N/OD	2014					X		[30]
59	Makhoba & Eric	CP	2010	X	X					[70]
60	McLaughlan	R	2006	X	X	X		X		[114]
61	Merafe	N/OD	2015	X	X	X	X	X	X	[71]
62	Metallurgical industry	Other	n.d.	X	X			X	X	[72]
63	Mills	TCM	2011	X	X		X			[73]
64	Milne et al.	JA	2013					X	X	[102]
65	Monsen	CP	1998					X	X	[74]
66	Mosiane	N/OD	2007		X	X				[75]
67	NAPCA	N/OD	1970					X	X	[76]
68	National Treasury	N/OD	2016					X		[31]
69	National Treasury	N/OD	2017					X		[33]
70	Niemelä	CP	2004	X				X	X	[14]
71	Nkohla	T/D	2006				X			[77]
72	NPI	N/OD	1999					X	X	[78]
73	Olsen	CP	1998					X	X	[37]
74	Otani	JA	1974	X	X					[4]
75	Pan	CP	2015	X						[8]
76	Pan	CP	2015	X	X		X			[6]
77	Penttilä	TCM	2016	X	X		X			[79]
78	Person	CP	1983					X		[80]
79	Pezennec	CP	2007					X		[81]
80	PMR	TCM	2013					X	X	[110]
81	Sri Sai Manasa Nature Tech	TCM	2017					X		[82]
82	Ranganathan	CP	2007	X	X					[42]
83	Riekkola-Vanhanen	N/OD	1999	X	X			X		[3]
84	Roos	CP	2004	X	X		X			[1]
85	Rudolph	R	1979					X		[115]
86	Scheepers	JA	2010		X		X			[83]
87	Segura	JA	2017	X	X		X			[84]
88	Sonntag-O'Brien	TCM	2000					X	X	[103]
89	Taggart	JA	2016		X			X		[85]
90	The iron and steel institute	B	2012		X		X			[116]
91	The Norwegian Emission Inv.	N/OD	2016					X	X	[109]
92	UNFCCC Reporting Guidel.	N/OD	2008					X	X	[17]
93	US EPA	N/OD	1992		X			X	X	[86]
94	Vaish	Other	1992		X			X	X	[87]
95	Visagie	R	2006	X		X				[88]
96	Visser	JA	2006		X					[40]
97	Weitz	T/D	2015	X	X		X	X	X	[47]
98	Westbrook & Dougherty	JA	1981					X		[117]
99	Xiao	CP	2006		X					[2]
100	Xstrata	N/OD	2011		X	X		X		[89]
101	Yang	CP	2004		X		X			[41]
102	Young	R	2010					X	X	[104]
103	Zayakin	CP	2015		X					[90]

PHASE 2:

Table A-3: Reference type distribution (Phase 2)

Type of reference	Percentage	Number
Journal article	8%	3
Conference paper	19%	7
Thesis / dissertation	6%	2
National official documentation	33%	12
Book	0%	0
Report	22%	8
Training course material	6%	2
Other	6%	2
Total	**100%**	**36**

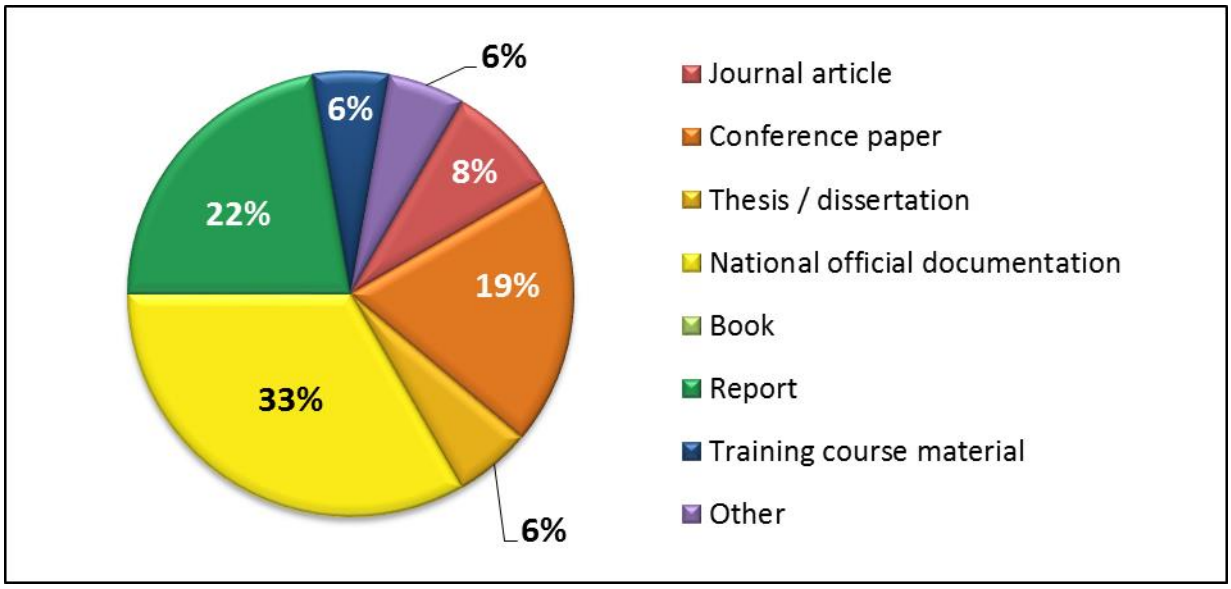


Figure A-2: Reference type distribution (Phase 2)

(A) *How should one quantify CO_2e GHG emissions for FeCr production?*

(B) *Are there practical examples available of FeCr emission calculations?*

(C) *How can one be sure that the final result is correct?*

(D) *How do the methods ("tiers") differ from each other; which one is the best? Other options?*

(E) *How would the different furnace technology influence the emissions / performance?*

(F) *Is it worthwhile to go through this much trouble, e.g. MB? (Cost vs accuracy vs complexity)*

Table A-4: Phase 2 of critical literature review

Reference	Type of ref.	Does reference address the following uncertainty?						Ref. nr. *(ref. list)*
		(A)	*(B)*	*(C)*	*(D)*	*(E)*	*(F)*	
ADEME	N/OD							[93]
APTA	N/OD							[94]
Booysen	JA	X						[22]
CAPCOA	N/OD							[95]
Chen & Johnson	R							[96]
Chesnokov	JA							[52]
Defra	R							[97]
Dept. of environmental affairs	N/OD	X		X				[19]
Dept. of environmental affairs	R	X						[32]
Environmental protection act	R	X						[107]
EPA	N/OD	X						[54]
Gous	T/D			X				[20]
Holappa	CP	X						[5]
IPCC	N/OD			X				[35]
IPCC	R	X						[99]
IPIECA	R							[100]
Koekemoer	CP	X						[67]
Lindstad	CP	X						[16]
Lindstad	CP	X						[38]
Merafe	N/OD	X						[71]
Metallurgical industry	Other	X						[72]
Milne et al.	JA	X						[102]
Monsen	CP	X						[74]
NAPCA	N/OD							[76]
Niemelä	CP	X						[14]
NPI	N/OD	X						[78]
Olsen	CP	X						[37]
PMR	TCM			X				[110]
Sonntag-O'Brien	TCM							[103]
The Norwegian Emission Inv.	N/OD	X						[109]
UNFCCC Reporting Guidel.	N/OD	X						[17]
US EPA	N/OD	X						[86]
Vaish	Other	X						[87]
Vellinga	R							[108]
Weitz	T/D	X						[47]
Young	R							[104]

B. APPENDIX B: General conversions and compositions

Table B-1: Typical proximate analyses of South African coal **[39]**

Coal (reductant) type	Ash	Volatiles	Fixed carbon
Anthracite	15%	6 - 10%	80%
Char	19%	1 - 2%	80%
Coke	16%	<1%	83%

Table B-2: Typical ultimate analyses of South African coal, dry base **[123, 124, 125]**

Reductant type	C	H	O	N	S
Anthracite	88.94%	3.40%	2.32%	1.55%	0.81%
Char	77.84%	0.34%	21.11%	0.71%	
Coke	89%	3.60%	0%	1.56%	4.95%

Table B-3: Typical chemical composition of fluxes in FeCr production **[126, 127, 128, 154]**

Flux type	Composition	
Dolomite	$CaMg(CO_3)_2$	100%
Limestone	$CaCO_3$	100%
Quartz	SiO_2	100%
Burnt lime	CaO	100%

Calculating the molecular weight of a material

$$MW_d = \sum_{x=1}^{12} \left(n_{x_d} \times MW_x\right)$$

Equation B-1: Molecular weight of material "d"

Where,

"MW" = Molecular weight

"d" = material, e.g. dolomite

"x" = specific element, e.g. Ca, Mg, C, O

"MW_d" = Molecular weight of material *"d"*

"n_{xd}" = number of atoms (from *"x"*) present in material *"d"*

"MW_x" = Molecular weight of element *"x"*

Calculating the amount of elements in a material

$$x_d = \frac{n_{x\,d} \times MW_x}{MW_d}$$

Equation B-2: Composition - amount of element ("x") present in material ("d")

Where *"x_d"* = Specific element (*"x"*) present in material (*"d"*).

Converting compound composition (mass percentage) to elemental composition

$$\%A = \frac{MW_A \times a}{MW_X} \times \%X$$

Equation B-3: Converting compound X composition to individual element (A) composition

$$\%B = \frac{MW_B \times b}{MW_X} \times \%X$$

Equation B-4: Converting compound X composition to individual element (B) composition

Where,

"%X" = Mass composition percentage of compound X

"%A" = Mass composition percentage of element A

"%B" = Mass composition percentage of element B

"a" = Number of molecules per element A in compound X

"b" = Number of molecules per element B in compound X

"MW_A" = Molecular weight of element A, in g/mol

"MW_B" = Molecular weight of element B, in g/mol

"MW_X" = Molecular weight of compound X, in g/mol

**Note that %A + %B must be equal to %X*

Converting volume percentage composition to mass percentage composition

$$Mass\ \% = \rho\left\{\frac{kg}{m^3}\right\} \times Volume\ \%$$

Equation B-5: Converting volume percentage composition to mass percentage composition

Where *"Mass %"* = Composition in mass percentage

"ρ" = Density, in kg/m^3

"Volume %" = Composition in volume percentage

Table B-4: Calculated mass composition of fluxes (element-based)

Material	Ca	Mg	C	O	Si
Dolomite	22%	13%	13%	52%	-
Limestone	40%	-	12%	48%	-
Quartz	-	-	-	53%	47%
Burnt lime	71%	-	-	29%	-

Table B-5: Typical chemical composition of chromite ore **[7]**

Ore composition	
Cr_2O_3	50%
FeO	25%
MgO	9%
Al_2O_3	10%
SiO_2	5%
CaO	1%

Table B-6: Calculated mass composition of chromite ore (element-based)

Composition		Cr	O	Fe	Mg	Al	Si	Ca
Cr_2O_3	50%	68%	32%	-	-	-	-	-
Fe_2O_3	25%	-	30%	70%	-	-	-	-
MgO	9%	-	40%	-	60%	-	-	-
Al_2O_3	10%	-	48%	-	-	52%	-	-
SiO_2	5%	-	53%	-	-	-	47%	-
CaO	1%	-	29%	-	-	-	-	71%
Total ore composition		**34.2%**	**34.6%**	**17.5%**	**5.4%**	**5.2%**	**2.3%**	**0.7%**

Table B-7: Typical mass composition of FeCr metal (element-based) **[7]**

FeCr metal composition	
Cr	56.7%
C	7.2%
Si	2.3%
Fe	33.8%

Table B-8: Typical chemical composition of slag by-product **[77]**

Slag composition	
SiO_2	23.2%
Al_2O_3	24.7%
MgO	19.8%
CaO	3.0%
FeO	10.7%
Cr_2O_3	18.6%

Table B-9: Calculated mass composition of slag by-product (element-based)

Composition		Cr	O	Fe	Mg	Al	Si	Ca
SiO_2	23.2%	-	53%	-	-	-	47%	-
Al_2O_3	24.7%	-	48%	-	-	52%	-	-
MgO	19.8%	-	40%	-	60%	-	-	-
CaO	3.0%	-	29%	-	-	-	-	71%
FeO	10.7%	-	22%	78%	-	-	-	-
Cr_2O_3	18.6%	68%	32%	-	-	-	-	-
Total slag composition		**12.7%**	**41.3%**	**8.3%**	**11.9%**	**12.8%**	**10.8%**	**2.1%**

Table B-10: Typical chemical composition of off-gas from FeCr production **[14, 15]**

Off-gas composition	
CO	75 - 90%
CO_2	2 - 10%
H_2	2 - 15%
N_2	2 - 7%

Table B-11: Calculated mass composition of off-gas from FeCr production (element-based)

Composition		C	O	H	N
CO	75 - 90%	43%	57%	0%	0%
CO_2	2 - 10%	27%	73%	0%	0%
H_2	2 - 15%	0%	0%	100%	0%
N_2	2 - 7%	0%	0%	0%	100%
Total off-gas composition		**33 - 41%**	**44 - 59%**	**2 - 15%**	**2 - 7%**

C. APPENDIX C: Elemental coal composition guide

Table C-1: Original coal Bulletin 113 data (proximate, ultimate, and ash analysis)

COLLIERY	PRODUCT	PROXIMATE ANALYSIS				ULTIMATE ANALYSIS						ASH ANALYSIS									
		Moist	Ash	VM	FC	C	H	N	S	O	SiO_2	Al_2O_3	Fe_2O_3	P_2O_5	TiO_2	CaO	MgO	K_2O	Na_2O	SO_3
		%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%
MPUMALANGA																				
Witbank - Middelburg - Secunda																				
Bituminous																				
Amot	Unwashed: Crushed coal	4.5	23.2	22.5	49.8	59.48	3.04	1.39	0.77	7.62	55.7	23.9	5.57	0.21	1.42	6.53	2.76	0.41	0.22	2.50
Arthur Taylor	Washed: Export small	2.8	12.4	27.0	57.8	70.77	4.11	1.69	0.58	7.65	47.4	30.5	4.64	1.04	1.62	7.23	2.21	0.44	0.18	3.56
ATCOM	Washed: Grade 1	2.8	14.6	26.6	56.0	70.15	3.78	1.49	0.96	6.82	41.6	26.8	10.2	2.21	1.34	9.18	2.21	0.45	0.31	4.06
	Grade 3	2.6	14.2	28.2	55.0	70.14	3.77	1.51	0.54	6.64	53.8	29.3	3.66	1.01	1.84	4.72	1.78	0.44	0.18	2.63
Bank 2	Washed: Power station small	2.9	15.9	23.5	57.7	67.83	3.79	1.57	0.53	7.48	46.2	33.6	3.65	1.56	1.58	7.36	1.72	0.51	0.10	2.40
	Low ash	2.9	7.6	30.0	59.5	74.94	4.36	1.85	0.47	7.88	40.6	32.4	7.07	2.53	2.11	8.32	1.41	0.86	0.15	3.61
Bank 5	Washed: Large nut	3.4	11.3	32.8	52.5	71.99	4.53	1.72	0.79	6.27	65.0	23.5	4.11	0.14	1.27	1.53	1.01	1.63	0.18	1.14
Blackwattle	Washed: Pea	3.0	14.6	24.7	57.7	69.82	3.64	1.58	0.41	6.95	50.4	38.1	2.68	1.04	2.00	2.53	0.39	0.51	0.06	0.59
Blesboklaagte	Unwashed: Top Seam	3.4	10.8	30.6	55.2	71.46	4.35	1.66	1.39	6.94	46.9	35.0	13.4	0.37	1.95	0.47	0.26	0.97	0.08	0.31
	Unwashed: Lower Seam	1.7	24.6	23.7	50.0	62.27	3.55	1.22	0.89	5.77	58.2	34.9	3.35	0.13	1.76	0.13	0.12	0.82	0.05	0.13
Boschmans	Washed: Pea	3.1	16.1	27.0	53.8	67.19	3.71	1.59	0.88	7.43	43.7	22.8	5.52	4.32	1.98	13.6	3.45	0.54	0.19	2.50
	Cyclone	3.3	13.6	26.1	57.0	69.52	3.66	1.67	0.66	7.59	48.7	27.1	2.88	3.38	1.82	9.12	2.04	0.50	0.19	2.50
Delmas	Washed: C Grade: Pea	4.2	16.1	24.3	55.4	65.25	3.55	1.54	0.78	8.58	43.9	33.3	3.49	1.32	1.30	8.19	1.80	0.50	0.64	4.32
	Washed: D Grade: Pea	4.5	16.4	26.4	52.7	64.93	3.55	1.55	0.61	8.46	41.6	33.8	2.76	1.92	1.33	10.5	1.67	0.46	0.41	4.18
Duvha	Blended : Crushed coal	2.3	30.3	20.6	46.8	56.78	3.02	1.27	0.97	5.36	55.2	28.6	5.22	0.64	1.66	3.11	1.07	0.90	0.10	1.86
Eikeboom (Section of Optimum)	Washed: High phosphorus: Pea	3.6	13.5	25.8	57.1	69.20	3.71	1.65	0.41	7.93	57.2	34.2	1.19	1.80	1.50	2.49	0.16	0.40	0.08	0.40
	Washed: Low phosphorus: Pea	3.2	10.7	30.5	55.6	71.09	4.34	1.74	0.34	8.59	57.3	34.0	3.94	0.17	1.33	0.59	0.27	0.45	0.09	0.33
Elandsfontein: No. 4 Seam	Washed: High phosphorus: Pea	3.1	11.9	24.1	60.9	71.91	3.76	1.71	0.60	7.02	47.3	34.9	1.59	1.22	1.85	6.95	0.72	0.70	0.30	2.61
	Washed: Low phosphorus: Small nut	2.7	13.2	27.2	56.9	71.75	4.04	1.50	0.39	6.42	62.4	32.5	1.38	0.09	1.93	0.40	0.24	0.44	0.12	0.43
Forzando	Washed: Export	3.8	11.3	31.6	53.3	69.13	4.40	1.66	0.76	8.95	47.5	26.4	6.54	0.26	1.26	8.36	2.02	0.57	0.28	6.39
Goedehoop	Washed: Goedehoop	2.6	13.8	25.4	58.2	69.69	4.15	1.39	0.63	7.74	40.6	28.9	7.42	2.24	1.54	10.6	2.45	0.41	0.47	5.30
	Anglo	2.4	15.6	24.6	57.4	68.69	3.99	1.60	0.61	7.11	49.4	27.7	3.40	1.51	1.60	7.98	2.52	0.47	0.32	4.30
	Low ash	2.5	7.2	32.4	57.9	76.02	4.74	1.82	0.65	7.07	38.0	32.1	5.27	2.80	1.80	11.5	2.18	0.58	0.46	4.41
Graspan: No 2 Seam	Washed: Small nut	3.7	17.6	26.1	52.6	66.67	3.30	1.50	0.43	6.80	42.4	30.7	3.69	0.95	1.54	10.8	2.71	0.55	0.07	5.91
No 1 Seam	Washed: Small nut	3.2	15.5	26.2	55.1	68.80	3.72	1.55	0.43	6.80	54.0	32.0	2.33	0.16	1.60	4.62	1.18	0.64	0.06	3.21
Greenside	Washed: Greenside	2.4	13.2	25.7	58.7	71.22	3.97	1.58	0.53	7.10	46.4	31.5	3.08	1.88	1.90	8.68	1.27	0.56	0.08	3.39
	Power station small	2.4	14.9	24.3	58.4	69.45	3.86	1.61	0.47	7.31	52.0	32.1	4.14	0.81	1.48	4.83	1.33	0.38	0.13	1.24
Inkhwezi	Unwashed: Run of mine	3.2	26.2	25.5	45.1	55.94	3.03	1.29	1.06	9.28	49.3	29.2	4.92	0.52	1.37	7.66	1.73	0.55	0.21	4.49
Khutala	Unwashed: Crushed coal	3.4	33.0	21.1	42.5	51.25	2.68	1.21	0.99	7.47	51.3	31.3	4.69	0.75	1.58	4.91	1.85	0.97	0.19	1.93
Kleinkopje	Washed: Anglo	2.8	15.4	24.0	57.8	68.88	3.77	1.54	0.69	6.92	45.6	37.1	3.83	1.29	1.60	5.67	1.11	0.53	0.15	2.61
Koornfontein	Washed: Export	2.8	13.2	26.3	57.7	70.36	4.07	1.55	0.63	7.39	41.9	34.0	2.57	1.62	1.60	8.74	2.29	0.56	0.18	5.18
Kriel: Opencast	Unwashed: Crushed coal	4.9	30.4	21.9	42.8	50.99	2.76	1.25	0.72	8.98	55.0	23.3	3.90	0.96	1.65	8.17	1.28	0.95	0.14	2.88
Undergrround	Unwashed: Crushed coal	4.3	23.1	23.8	48.8	57.92	2.96	1.42	0.93	9.35	45.5	25.2	4.28	0.93	1.63	13.0	2.68	0.92	0.51	4.15
Lakeside	Washed: Pea	4.4	11.6	26.0	58.0	69.44	3.62	1.66	0.38	8.90	40.4	36.4	1.61	2.24	1.87	9.12	2.22	0.76	0.14	4.47
Landau (Kromdraai)	Washed: Power station small	2.8	14.2	23.8	59.2	69.34	3.95	1.55	0.59	7.57	50.5	42.1	2.00	1.03	2.04	1.03	0.18	0.48	0.06	0.57
Leeuwfontein: Opencast	Pea	4.2	13.8	23.9	58.1	68.69	3.48	1.49	0.36	7.98	54.8	34.4	2.42	1.21	1.43	3.15	0.22	0.37	0.08	0.96
Undergrround	Washed: Pea	4.5	11.6	29.4	54.5	68.94	3.83	1.52	0.37	9.24	49.7	27.4	2.49	0.49	1.38	10.3	2.61	0.41	0.23	4.23
Leeuwpan	Washed: Small nut	2.9	14.1	24.6	58.4	68.53	3.59	1.59	0.64	8.65	40.9	33.5	3.29	0.54	1.71	8.34	2.33	1.00	1.36	6.91
Leeuwspruit	Washed: 50 x 0mm	2.6	13.8	28.8	54.8	70.83	4.03	1.62	0.81	6.31	36.5	33.9	5.80	3.56	1.58	10.0	1.46	0.81	0.14	4.31
Lemoenfontein	Unwashed: Run of mine	3.8	8.3	33.6	54.3	72.80	4.58	1.72	1.65	7.15	46.0	27.8	20.4	0.37	1.36	0.86	0.35	0.32	0.09	1.31
Matla	Unwashed: Crushed coal	5.3	27.1	24.1	43.5	52.71	2.91	1.29	1.08	9.61	48.2	26.4	4.33	0.98	1.51	9.71	1.93	0.77	0.46	4.31
Middelburg Consolidated	Washed: Small	2.5	14.1	24.2	59.2	70.25	3.77	1.57	0.45	7.37	50.5	34.8	2.44	1.33	1.82	4.68	1.25	0.65	0.08	1.33
New Clydesdale	Washed: Low ash	2.6	6.8	31.2	59.4	75.99	4.59	1.74	0.57	7.71	40.8	33.4	5.58	1.67	1.68	7.71	2.14	0.93	0.22	4.99

COLLIERY	PRODUCT		PROXIMATE ANALYSIS				ULTIMATE ANALYSIS					ASH ANALYSIS									
			Moist	Ash	VM	FC	C	H	N	S	O	SiO2	Al2O3	Fe2O3	P2O5	TiO2	CaO	MgO	K2O	Na2O	SO3
			%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%
MPUMALANGA																					
Witbank - Middelburg - Secunda																					
Bituminous																					
New Denmark	Unwashed:	Crushed coal	3.5	31.6	21.9	43.0	52.08	2.80	1.40	1.25	7.37	55.5	26.2	6.98	0.19	1.34	3.23	1.21	1.22	0.40	1.96
Olifantslaagte	Washed:	Pea	5.0	13.4	24.0	57.6	67.16	3.71	1.58	0.24	8.91	49.8	39.3	1.38	2.35	1.10	2.93	0.55	0.72	0.12	1.09
Optimum	Washed:	Optimum	3.2	10.5	32.4	53.9	71.61	4.28	1.72	0.65	8.04	51.2	34.2	2.49	1.20	1.22	5.02	1.35	0.43	0.15	1.84
	Blended :	Power station small	3.6	22.9	23.4	50.1	60.64	3.32	1.36	0.58	7.60	55.9	27.6	3.25	0.76	1.44	4.74	2.13	0.51	0.30	2.51
Phoenix	Washed:	Pea	2.7	15.8	26.6	54.9	69.06	3.63	1.35	0.30	7.16	56.3	28.4	3.17	0.18	1.42	4.10	1.95	0.41	0.36	2.31
Polmaise	Washed:	Small	3.0	11.2	25.9	59.9	72.78	4.06	1.81	0.54	6.61	50.0	38.5	4.95	0.97	1.81	1.63	0.40	0.81	0.05	0.79
Rietspruit	Washed:	Small	3.1	13.8	26.9	56.2	69.74	4.05	1.58	0.65	7.08	47.2	29.9	4.28	1.61	1.41	8.16	2.22	0.48	0.11	4.06
Secunda: Bosjesspruit	Unwashed:	Crushed coal	3.9	32.8	21.6	41.7	50.48	2.74	1.23	1.61	7.24	57.0	23.3	5.75	0.30	1.09	4.86	1.68	1.05	0.44	3.22
Middelbult	Unwashed:	Crushed coal	4.2	23.8	22.7	49.3	58.31	2.98	1.44	1.12	8.15	48.6	25.6	4.57	0.81	1.72	8.69	2.90	0.54	0.57	4.69
Brandspruit	Unwashed:	Crushed coal	4.4	23.8	22.6	49.2	56.25	2.87	1.52	1.04	10.12	44.4	30.7	3.67	0.93	1.81	7.82	2.75	0.94	0.48	5.04
Syferfontein	Unwashed:	Crushed coal	5.6	28.3	22.0	44.1	52.18	2.75	1.30	0.75	9.12	54.6	24.4	4.35	0.53	1.54	6.27	2.28	0.87	0.47	3.57
Twistdraai	Washed:	Export	4.1	9.4	32.7	53.8	70.09	4.44	1.83	0.86	9.28	38.8	32.5	4.91	1.51	2.11	9.57	3.18	0.67	0.67	5.01
		Middling	3.3	37.1	21.6	38.0	47.08	2.61	1.09	1.36	7.46	53.4	29.7	3.92	0.58	1.59	3.59	1.39	1.19	0.35	2.36
South Witbank		Pea	3.7	16.0	28.2	52.1	66.61	3.77	1.58	0.96	7.38	47.0	29.8	3.79	2.08	1.74	10.5	1.87	0.51	0.28	2.41
Leeuwpan (Stuart)	Washed:	Pea	3.2	20.1	29.1	47.6	62.72	3.95	1.47	0.49	8.07	51.0	38.2	1.68	0.31	1.88	3.42	0.93	0.74	0.16	1.31
Tavistock: No. 4 Seam	Washed:	Pea	3.4	11.3	27.3	58.0	71.43	3.89	1.70	0.66	7.62	44.8	26.5	3.07	2.40	1.75	13.2	3.52	0.43	0.14	4.18
Van Dyks Drift	Washed:	Pea	2.5	13.8	25.8	57.9	71.37	3.96	1.66	0.59	6.12	45.7	31.2	4.26	2.19	1.35	9.36	1.77	0.69	0.11	3.31
		Low ash	2.4	6.9	31.8	58.9	76.13	4.82	1.80	0.64	7.31	42.9	33.3	4.87	2.03	2.11	7.92	1.83	0.76	0.26	3.03
		Premium	2.5	13.7	25.5	58.3	70.47	3.98	1.58	0.58	7.19	46.5	30.8	4.31	1.79	1.41	9.02	1.52	0.53	0.18	2.20
		Premuim	2.5	14.6	24.4	58.5	69.88	3.96	1.51	0.52	7.03	46.4	28.6	5.28	2.07	1.61	9.51	1.82	0.58	0.11	3.61
Waterpan	Washed:	Export	3.4	11.6	27.4	57.6	72.00	3.72	1.78	0.57	6.93	54.7	26.4	4.17	2.08	1.58	6.86	1.54	0.46	0.13	1.39
Witbank Consolidated	Washed:	Pea (Norwalt)	3.0	14.4	27.1	55.5	69.14	3.68	1.62	1.05	7.11	35.8	26.5	9.63	2.14	1.41	13.9	3.63	0.70	0.23	5.50
	Washed:	Cyclone	3.3	13.8	24.2	58.7	69.96	3.51	1.64	0.43	7.36	42.4	34.1	2.93	1.76	2.15	8.32	2.69	0.68	0.22	4.11
Woestalleen	Washed:	Low phosphorus: Small nut	4.0	12.1	25.6	58.3	70.35	3.74	1.67	0.64	7.50	57.9	32.4	4.18	0.19	1.61	0.44	0.30	0.74	0.04	0.37
Belfast - Carolina - Ermelo																					
Bituminous																					
Coastal Fuels: (Paardeplaats Section)	Unwashed:	Pea	2.9	10.6	36.2	50.3	71.17	4.70	1.74	1.09	7.80	53.1	28.8	11.60	0.30	1.48	1.63	0.62	0.47	0.15	1.59
(Witkrans Section)	Unwashed:	Small nut	2.5	17.1	29.7	50.7	66.34	4.14	1.60	0.57	7.75	60.7	33.5	1.84	0.20	1.55	0.56	0.30	0.68	0.06	0.16
Delta	Washed:	Pea	2.9	13.5	28.2	55.4	69.52	4.05	1.82	0.90	7.31	51.5	27.0	6.85	0.34	1.48	3.98	1.85	1.00	0.60	3.91
Eastside	Unwashed:	Nut	2.8	8.7	33.2	55.3	73.90	4.70	1.88	0.69	7.33	51.5	34.4	4.30	0.32	1.49	3.41	1.38	0.59	0.26	1.74
Glisa	Unwashed:	Pea	4.1	18.6	22.8	54.5	62.46	3.20	1.46	0.85	9.33	40.0	34.5	6.93	0.55	1.91	8.84	3.69	0.38	0.20	2.47
Golfview	Washed:	Prime: Pea	3.5	11.3	33.5	51.7	69.27	4.41	2.00	0.79	8.73	46.1	28.2	7.44	0.30	1.20	6.69	2.03	0.45	0.51	5.40
	Washed:	Middling: Pea	3.8	18.9	26.8	50.5	62.95	3.50	1.74	0.84	8.27	50.4	28.1	5.85	0.21	1.13	4.69	1.84	0.51	0.30	4.96
Spitzkop	Washed:	Pea	3.1	14.3	30.1	52.5	68.65	4.13	1.71	1.14	6.98	47.8	26.5	8.95	0.32	1.43	5.48	1.73	0.74	0.60	1.91
		Export	3.0	13.6	30.7	52.7	68.94	4.36	1.68	1.29	7.13	45.6	30.0	8.29	0.33	1.33	5.25	1.95	0.55	0.33	5.70
Strathrae	Washed:	Pea	4.0	14.3	24.2	57.5	67.99	3.46	1.61	0.65	7.99	50.6	26.7	5.78	0.75	1.41	6.46	2.64	0.36	0.19	4.61
Sumo	Washed:	Pea	5.4	13.1	22.8	58.7	68.52	3.36	1.58	0.33	7.71	49.7	26.2	7.66	1.55	1.30	5.86	1.30	1.10	0.89	3.27
Tselentis (Bothasrust)	Washed:	Pea	3.2	14.7	26.5	55.6	69.39	3.86	1.48	0.56	6.81	57.3	26.3	3.77	1.29	1.52	3.94	1.32	0.77	0.11	2.64

COLLIERY	PRODUCT		PROXIMATE ANALYSIS				ULTIMATE ANALYSIS					ASH ANALYSIS									
			Moist	Ash	VM	FC	C	H	N	S	O	SiO2	Al2O3	Fe2O3	P2O5	TiO2	CaO	MgO	K2O	Na2O	SO3
			%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%	%
Piet Retief - Wakkerstroom																					
Anthracitic																					
Protea	Washed:	Pea	3.2	18.4	6.0	72.4	73.92	2.07	1.31	0.68	0.42	48.5	22.60	7.54	0.32	1.57	5.25	3.00	1.57	5.23	4.69
Bituminous																					
Savmore (Maquassa)	Washed:	Pea	3.7	12.8	28.5	55.0	69.70	3.69	1.87	1.40	6.84	36.8	19.20	14.30	1.05	1.18	14.00	2.91	0.50	0.25	9.10
TBS	Washed:	Pea	4.4	14.2	32.6	48.8	65.89	4.27	1.73	0.98	8.53	50	33.60	6.96	0.17	1.44	3.51	1.07	0.70	0.20	1.98
Kangwane (Komatipoort)																					
Anthracitic																					
Nkomati Anthracite	Washed:	Pea	1.5	14.7	7.8	76.0	78.40	2.58	1.62	0.35	0.85	50.1	27.10	6.60	0.29	1.28	6.93	2.27	0.44	0.63	4.26
NORTHERN PROVINCE																					
Ellisras																					
Bituminous																					
Grootegeluk	Washed:	Pea	2.8	15.8	23.5	57.9	68.17	3.99	1.28	0.58	7.38	52.5	35.80	0.99	0.35	1.63	3.54	1.58	0.32	0.15	2.72
		Coking	3.3	9.8	35.7	51.2	72.23	4.70	1.46	0.86	7.65	67.2	19.40	5.34	0.21	1.73	1.36	0.59	0.99	0.24	1.02
		Middling	2.5	33.8	26.7	37.0	50.89	3.36	1.00	1.48	6.97	62.5	21.80	8.22	0.33	0.92	2.35	0.83	0.87	0.18	1.85
Venda																					
Bituminous																					
Tshikondeni	Washed:	Coking	0.8	12.5	23.7	63.0	78.41	4.23	1.60	0.94	1.53	57	25.00	4.96	0.48	1.40	3.38	1.69	1.40	0.64	3.55
FREE STATE																					
Sasolburg																					
Bituminous																					
New Vaal	Washed:	Crushed coal	5.9	40.2	22.3	31.6	40.90	2.43	0.95	0.55	9.07	57.6	31.70	2.61	0.25	1.55	2.50	0.76	0.44	0.19	1.44
Sigma	Unwashed:	+6mm	6.2	31.5	21.9	40.4	49.73	2.50	1.21	0.93	7.93	53.8	25.60	6.49	0.27	1.51	6.23	1.55	0.43	0.35	3.57
KWAZULU-NATAL																					
Dundee - Newcastle - Utrecht																					
Anthracitic																					
CBR Mining	Washed:	Pea	2.0	12.8	10.9	74.3	75.79	3.13	2.04	1.34	2.90	50	31.90	10.01	0.78	1.42	1.33	0.77	1.33	1.80	0.78
Springlake	Washed:	Pea	1.7	12.3	10.3	75.7	77.80	3.25	2.06	1.55	1.34	48	34.90	5.24	0.80	1.69	3.43	0.64	1.78	0.88	1.93
Bituminous																					
CBR Mining	Washed:	Pea	1.9	17.0	16.5	64.6	71.40	3.37	1.92	1.60	2.81	45	28.40	5.51	0.67	1.59	8.19	1.82	1.44	1.94	4.12
Durban Navigation	Washed:	Coking	1.5	11.5	30.1	56.9	74.69	4.75	2.00	1.46	4.10	46	30.90	8.46	0.87	1.59	5.45	1.09	1.59	0.92	2.74
Welgedacht	Washed:	Small pea	3.1	13.9	28.0	55.0	69.76	4.03	1.81	1.53	5.87	42	24.10	11.70	0.65	1.43	9.75	2.07	0.85	1.05	6.86
Vryheid																					
Anthracitic																					
Duiker																					
- Dixon: Gus Seam	Washed:	8 x 0.5mm	3.3	12.0	5.2	79.5	78.93	2.15	1.64	0.90	1.08	50	29.30	8.36	0.29	2.02	1.87	1.27	2.09	2.54	1.01
- Enyati: Alfred Seam	Washed:	8 x 0.5mm	3.0	13.9	5.4	77.7	77.44	2.05	1.77	0.89	0.95	44	32.80	4.94	2.18	2.06	7.43	1.98	0.85	0.19	3.27
- Oakhurst Section	Washed:	45 x 22 mm	2.1	12.5	9.8	75.6	78.90	3.03	2.23	0.74	0.50	55	29.40	5.37	0.29	1.67	1.04	1.07	2.56	1.90	0.94
- Heritage: Dundas Seam	Washed:	19 x 10 mm	2.8	16.3	7.4	73.5	73.90	2.53	1.77	0.53	2.17	45	28.50	5.02	1.25	1.49	8.79	2.10	1.66	1.95	3.01
- Rietvlei Section	Washed:	8 x 0.5mm	4.1	11.8	5.5	78.6	78.32	2.35	1.89	1.25	0.29	49	29.30	9.63	0.28	2.03	1.33	1.20	2.52	1.93	0.92
Bituminous																					
Recmin	Unwashed:	NAC fines	3.9	24.8	13.0	58.3	61.85	2.90	1.75	0.69	4.11	52	21.70	17.50	0.47	1.76	0.92	0.75	2.77	0.41	1.20
Vryheid Coronation	Washed:	Coking	1.0	12.0	20.2	66.8	79.05	3.98	1.86	0.70	1.41	52	34.00	5.33	0.16	1.96	0.71	0.45	2.56	0.49	0.87
Ulundi																					
Antracitic																					
Zululand Anthracite	Washed:	20 x 6.3mm	2.8	8.1	6.0	83.1	83.32	2.60	1.84	0.80	0.54	45	28.50	14.20	0.84	1.66	3.19	1.00	2.82	0.41	1.21
		Middling	3.0	24.7	7.7	64.6	66.58	2.01	1.40	1.50	0.81	50	19.60	12.50	0.35	1.01	8.66	1.35	2.40	0.38	2.89
SWAZILAND																					
Antracitic																					
Maloma	Washed:	Pea	1.8	9.9	6.1	82.2	82.04	2.89	1.94	0.64	0.79	56	28.60	3.07	0.17	1.65	2.91	1.10	1.50	1.85	2.04

Table C-2: Total elemental coal composition

Colliery	Coal elemental composition (incl. moisture)						Coal elemental composition (dry base)					
	C (%)	H (%)	O (%)	N (%)	S (%)	*Trace* (%)	C (%)	H (%)	O (%)	N (%)	S (%)	*Trace* (%)
MPUMALANGA												
Witbank - Middelburg - Secunda												
Bituminous												
Arnot	59.5	3.54	11.6	1.39	0.77	23.20	62.3	3.18	8.0	1.46	0.81	24.29
Arthur Taylor	70.8	4.42	10.1	1.69	0.58	12.40	72.8	4.23	7.9	1.74	0.60	12.76
ATCOM	70.2	4.09	9.3	1.49	0.96	14.60	71.7	3.87	7.0	1.52	0.98	14.93
	70.1	4.06	8.9	1.51	0.54	14.20	72.5	3.89	6.9	1.56	0.56	14.67
Bank 2	67.8	4.12	10.1	1.57	0.53	15.90	69.9	3.90	7.7	1.62	0.55	16.37
	74.9	4.69	10.5	1.85	0.47	7.60	77.2	4.49	8.1	1.91	0.48	7.83
Bank 5	72.0	4.91	9.3	1.72	0.79	11.30	74.5	4.69	6.5	1.78	0.82	11.70
Blackwattle	69.8	3.98	9.6	1.58	0.41	14.60	72.0	3.75	7.2	1.63	0.42	15.05
Blesboklaagte	71.5	4.73	10.0	1.66	1.39	10.80	74.0	4.50	7.2	1.72	1.44	11.18
	62.3	3.74	7.3	1.22	0.89	24.60	63.3	3.61	5.9	1.24	0.91	25.03
Boschmans	67.2	4.06	10.2	1.59	0.88	16.10	69.3	3.83	7.7	1.64	0.91	16.62
	69.5	4.03	10.5	1.67	0.66	13.60	71.9	3.78	7.8	1.73	0.68	14.06
Delmas	65.3	4.02	12.3	1.54	0.78	16.10	68.1	3.71	9.0	1.61	0.81	16.81
	64.9	4.05	12.5	1.55	0.61	16.40	68.0	3.72	8.9	1.62	0.64	17.17
Duvha	56.8	3.28	7.4	1.27	0.97	30.30	58.1	3.09	5.5	1.30	0.99	31.01
Eikeboom (Section of Optimum)	69.2	4.11	11.1	1.65	0.41	13.50	71.8	3.85	8.2	1.71	0.43	14.00
	71.1	4.70	11.4	1.74	0.34	10.70	73.4	4.48	8.9	1.80	0.35	11.05
Elandsfontein: No. 4 Seam	71.9	4.11	9.8	1.71	0.60	11.90	74.2	3.88	7.2	1.76	0.62	12.28
	71.8	4.34	8.8	1.50	0.39	13.20	73.7	4.15	6.6	1.54	0.40	13.57
Forzando	69.1	4.83	12.3	1.66	0.76	11.30	71.9	4.57	9.3	1.73	0.79	11.75
Goedehoop	69.7	4.44	10.0	1.39	0.63	13.80	71.6	4.26	7.9	1.43	0.65	14.17
	68.7	4.26	9.2	1.60	0.61	15.60	70.4	4.09	7.3	1.64	0.63	15.98
	76.0	5.02	9.3	1.82	0.65	7.20	78.0	4.86	7.3	1.87	0.67	7.38
Graspan	66.7	3.71	10.1	1.50	0.43	17.60	69.2	3.43	7.1	1.56	0.45	18.28
	68.8	4.08	9.6	1.55	0.43	15.50	71.1	3.84	7.0	1.60	0.44	16.01
Greenside	71.2	4.24	9.2	1.58	0.53	13.20	73.0	4.07	7.3	1.62	0.54	13.52
	69.5	4.13	9.4	1.61	0.47	14.90	71.2	3.95	7.5	1.65	0.48	15.27
Inkhwezi	55.9	3.39	12.1	1.29	1.06	26.20	57.8	3.13	9.6	1.33	1.10	27.07
Khutala	51.3	3.06	10.5	1.21	0.99	33.00	53.1	2.77	7.7	1.25	1.02	34.16
Kleinkopje	68.9	4.08	9.4	1.54	0.69	15.40	70.9	3.88	7.1	1.58	0.71	15.84
Koornfontein	70.4	4.38	9.9	1.55	0.63	13.20	72.4	4.19	7.6	1.59	0.65	13.58
Kriel	51.0	3.31	13.3	1.25	0.72	30.40	53.6	2.90	9.4	1.31	0.76	31.97
	57.9	3.44	13.2	1.42	0.93	23.10	60.5	3.09	9.8	1.48	0.97	24.14
Lakeside	69.4	4.11	12.8	1.66	0.38	11.60	72.6	3.79	9.3	1.74	0.40	12.13
Landau (Kromdraai)	69.3	4.26	10.1	1.55	0.59	14.20	71.3	4.06	7.8	1.59	0.61	14.61
Leeuwfontein	68.7	3.95	11.7	1.49	0.36	13.80	71.7	3.63	8.3	1.56	0.38	14.41
	68.9	4.33	13.2	1.52	0.37	11.60	72.2	4.01	9.7	1.59	0.39	12.15
Leeuwpan	68.5	3.92	11.2	1.59	0.64	14.10	70.6	3.70	8.9	1.64	0.66	14.52
Leeuwspruit	70.8	4.32	8.6	1.62	0.81	13.80	72.7	4.14	6.5	1.66	0.83	14.17
Lemoenfontein	72.8	5.01	10.5	1.72	1.65	8.30	75.7	4.76	7.4	1.79	1.72	8.63
Matla	52.7	3.50	14.3	1.29	1.08	27.10	55.7	3.07	10.1	1.36	1.14	28.62

Colliery	Coal elemental composition (incl. moisture)						Coal elemental composition (dry base)					
	C (%)	H (%)	O (%)	N (%)	S (%)	*Trace* (%)	C (%)	H (%)	O (%)	N (%)	S (%)	*Trace* (%)
Middelburg Consolidated	70.3	4.05	9.6	1.57	0.45	14.10	72.0	3.87	7.6	1.61	0.46	14.46
New Clydesdale	76.0	4.88	10.0	1.74	0.57	6.80	78.0	4.71	7.9	1.79	0.59	6.98
New Denmark	52.1	3.19	10.5	1.40	1.25	31.60	54.0	2.90	7.6	1.45	1.30	32.75
Olifantslaagte	67.2	4.27	13.3	1.58	0.24	13.40	70.7	3.91	9.4	1.66	0.25	14.11
Optimum	71.6	4.64	10.9	1.72	0.65	10.50	74.0	4.42	8.3	1.78	0.67	10.85
	60.6	3.72	10.8	1.36	0.58	22.90	62.9	3.44	7.9	1.41	0.60	23.76
Phoenix	69.1	3.93	9.6	1.35	0.30	15.80	71.0	3.73	7.4	1.39	0.31	16.24
Polmaise	72.8	4.40	9.3	1.81	0.54	11.20	75.0	4.19	6.8	1.87	0.56	11.55
Rietspruit	69.7	4.40	9.8	1.58	0.65	13.80	72.0	4.18	7.3	1.63	0.67	14.24
Secunda: Bosjesspruit	50.5	3.18	10.7	1.23	1.61	32.80	52.5	2.85	7.5	1.28	1.68	34.13
Secunda: Middelbult	58.3	3.45	11.9	1.44	1.12	23.80	60.9	3.11	8.5	1.50	1.17	24.84
Secunda: Brandspruit	56.3	3.36	14.0	1.52	1.04	23.80	58.8	3.00	10.6	1.59	1.09	24.90
Secunda: Syferfontein	52.2	3.38	14.1	1.30	0.75	28.30	55.3	2.91	9.7	1.38	0.79	29.98
Secunda: Twistdraai	70.1	4.90	12.9	1.83	0.86	9.40	73.1	4.63	9.7	1.91	0.90	9.80
	47.1	2.98	10.4	1.09	1.36	37.10	48.7	2.70	7.7	1.13	1.41	38.37
South Witbank	66.6	4.18	10.7	1.58	0.96	16.00	69.2	3.91	7.7	1.64	1.00	16.61
Leeuwpan (Stuart)	62.7	4.31	10.9	1.47	0.49	20.10	64.8	4.08	8.3	1.52	0.51	20.76
Tavistock: No. 4 Seam	71.4	4.27	10.6	1.70	0.66	11.30	73.9	4.03	7.9	1.76	0.68	11.70
Van Dyks Drift	71.4	4.24	8.3	1.66	0.59	13.80	73.2	4.06	6.3	1.70	0.61	14.15
	76.1	5.09	9.4	1.80	0.64	6.90	78.0	4.94	7.5	1.84	0.66	7.07
	70.5	4.26	9.4	1.58	0.58	13.70	72.3	4.08	7.4	1.62	0.59	14.05
	69.9	4.24	9.2	1.51	0.52	14.60	71.7	4.06	7.2	1.55	0.53	14.97
Waterpan	72.0	4.10	9.9	1.78	0.57	11.60	74.5	3.85	7.2	1.84	0.59	12.01
Witbank	69.1	4.02	9.8	1.62	1.05	14.40	71.3	3.79	7.3	1.67	1.08	14.85
	70.0	3.88	10.3	1.64	0.43	13.80	72.3	3.63	7.6	1.70	0.44	14.27
Woestalleen	70.4	4.19	11.1	1.67	0.64	12.10	73.3	3.90	7.8	1.74	0.67	12.60
Belfast - Carolina - Ermelo												
Bituminous												
Coastal Fuels: Paardeplaats	71.2	5.03	10.4	1.74	1.09	10.60	73.3	4.84	8.0	1.79	1.12	10.92
Coastal Fuels: Witkrans	66.3	4.42	10.0	1.60	0.57	17.10	68.0	4.25	7.9	1.64	0.58	17.54
Delta	69.5	4.38	9.9	1.82	0.90	13.50	71.6	4.17	7.5	1.87	0.93	13.90
Eastside	73.9	5.01	9.8	1.88	0.69	8.70	76.0	4.84	7.5	1.93	0.71	8.95
Glisa	62.5	3.66	13.0	1.46	0.85	18.60	65.1	3.34	9.7	1.52	0.89	19.40
Golfview	69.3	4.80	11.8	2.00	0.79	11.30	71.8	4.57	9.0	2.07	0.82	11.71
	63.0	3.93	11.6	1.74	0.84	18.90	65.4	3.64	8.6	1.81	0.87	19.65
Spitzkop	68.7	4.48	9.7	1.71	1.14	14.30	70.8	4.26	7.2	1.76	1.18	14.76
	68.9	4.70	9.8	1.68	1.29	13.60	71.1	4.49	7.4	1.73	1.33	14.02
Strathrae	68.0	3.91	11.5	1.61	0.65	14.30	70.8	3.60	8.3	1.68	0.68	14.90
Sumo	68.5	3.97	12.5	1.58	0.33	13.10	72.4	3.55	8.2	1.67	0.35	13.85
Tselentis (Bothasrust)	69.4	4.22	9.7	1.48	0.56	14.70	71.7	3.99	7.0	1.53	0.58	15.19
Piet Retief - Wakkerstroom												
Anthracitic												
Protea	73.9	2.43	3.3	1.31	0.68	18.40	76.4	2.14	0.4	1.35	0.70	19.01
Bituminous												
Savmore	69.7	4.10	10.1	1.87	1.40	12.80	72.4	3.83	7.1	1.94	1.45	13.29
TBS	65.9	4.76	12.4	1.73	0.98	14.20	68.9	4.47	8.9	1.81	1.03	14.85

Colliery	Coal elemental composition (incl. moisture)						Coal elemental composition (dry base)					
	C (%)	H (%)	O (%)	N (%)	S (%)	*Trace* (%)	C (%)	H (%)	O (%)	N (%)	S (%)	*Trace* (%)
Kangwane (Komatipoort)												
Anthracitic												
Nkomati Anthracite	78.4	2.75	2.2	1.62	0.35	14.70	79.6	2.62	0.9	1.64	0.36	14.92
NORTHERN PROVINCE												
Ellisras												
Bituminous												
Grootegeluk	68.2	4.30	9.9	1.28	0.58	15.80	70.1	4.10	7.6	1.32	0.60	16.26
	72.2	5.07	10.6	1.46	0.86	9.80	74.7	4.86	7.9	1.51	0.89	10.13
	50.9	3.64	9.2	1.00	1.48	33.80	52.2	3.45	7.1	1.03	1.52	34.67
Venda												
Bituminous												
Tshikondeni	78.4	4.32	2.2	1.60	0.94	12.50	79.0	4.26	1.5	1.61	0.95	12.60
FREE STATE												
Sasolburg												
Bituminous												
New Vaal	40.9	3.09	14.3	0.95	0.55	40.20	43.5	2.58	9.6	1.01	0.58	42.72
Sigma	49.7	3.20	13.4	1.21	0.93	31.50	53.0	2.67	8.5	1.29	0.99	33.58
KWAZULU-NATAL												
Dundee - Newcastle - Utrecht												
Anthracitic												
CBR Mining	75.8	3.35	4.7	2.04	1.34	12.80	77.3	3.19	3.0	2.08	1.37	13.06
Springlake	77.8	3.44	2.8	2.06	1.55	12.30	79.1	3.31	1.4	2.10	1.58	12.51
Bituminous												
CBR Mining	71.4	3.58	4.5	1.92	1.60	17.00	72.8	3.44	2.9	1.96	1.63	17.33
Durban Navigation	74.7	4.92	5.4	2.00	1.46	11.50	75.8	4.82	4.2	2.03	1.48	11.68
Welgedacht	69.8	4.38	8.6	1.81	1.53	13.90	72.0	4.16	6.1	1.87	1.58	14.34
Vryheid												
Anthracitic												
Duiker: Dixon (Gus)	78.9	2.52	4.0	1.64	0.90	12.00	81.6	2.22	1.1	1.70	0.93	12.41
Duiker: Enyati (Alfred)	77.4	2.39	3.6	1.77	0.89	13.90	79.8	2.11	1.0	1.82	0.92	14.33
Duiker: Oakhurst	78.9	3.27	2.4	2.23	0.74	12.50	80.6	3.09	0.5	2.28	0.76	12.77
Duiker: Dundas Seam	73.9	2.84	4.7	1.77	0.53	16.30	76.0	2.60	2.2	1.82	0.55	16.77
Rietvlei	78.3	2.81	3.9	1.89	1.25	11.80	81.7	2.45	0.3	1.97	1.30	12.30
Bituminous												
Recmin	61.9	3.34	7.6	1.75	0.69	24.80	64.4	3.02	4.3	1.82	0.72	25.81
Vryheid Coronation	79.1	4.09	2.3	1.86	0.70	12.00	79.8	4.02	1.4	1.88	0.71	12.12
Ulundi												
Anthracitic												
Zululand Anthracite	83.3	2.91	3.0	1.84	0.80	8.10	85.7	2.67	0.6	1.89	0.82	8.33
	66.6	2.35	3.5	1.40	1.50	24.70	68.6	2.07	0.8	1.44	1.55	25.46
SWAZILAND												
Anthracitic												
Maloma	82.0	3.09	2.4	1.94	0.64	9.90	83.5	2.94	0.8	1.98	0.65	10.08

Table C-3: Proximate and ultimate analysis data (per coal field)

COLLIERY	PROXIMATE ANALYSIS				ULTIMATE ANALYSIS				
	Moisture	Ash	Volatile matter	Fixed carbon	C	H	N	S	O
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
MPUMALANGA									
Witbank - Middelburg - Secunda									
Bituminous									
Arnot	4.5	23.2	22.5	49.8	59.48	3.04	1.39	0.77	7.62
Arthur Taylor	2.8	12.4	27.0	57.8	70.77	4.11	1.69	0.58	7.65
ATCOM	2.7	14.4	27.4	55.5	70.1	3.8	1.5	0.8	6.7
Bank 2	2.9	11.8	26.8	58.6	71.4	4.1	1.7	0.5	7.7
Bank 5	3.4	11.3	32.8	52.5	71.99	4.53	1.72	0.79	6.27
Blackwattle	3.0	14.6	24.7	57.7	69.82	3.64	1.58	0.41	6.95
Blesboklaagte	2.6	17.7	27.2	52.6	66.9	4.0	1.4	1.1	6.4
Boschmans	3.2	14.9	26.6	55.4	68.4	3.7	1.6	0.8	7.5
Delmas	4.4	16.3	25.4	54.1	65.1	3.6	1.5	0.7	8.5
Duvha	2.3	30.3	20.6	46.8	56.78	3.02	1.27	0.97	5.36
Eikeboom (Section of Optimum)	3.4	12.1	28.2	56.4	70.1	4.0	1.7	0.4	8.3
Elandsfontein: No. 4 Seam	2.9	12.6	25.7	58.9	71.8	3.9	1.6	0.5	6.7
Forzando	3.8	11.3	31.6	53.3	69.13	4.40	1.66	0.76	8.95
Goedehoop	2.5	12.2	27.5	57.8	71.5	4.3	1.6	0.6	7.3
Graspan	3.5	16.6	26.2	53.9	67.7	3.5	1.5	0.4	6.8
Greenside	2.4	14.1	25.0	58.6	70.3	3.9	1.6	0.5	7.2
Inkhwezi	3.2	26.2	25.5	45.1	55.94	3.03	1.29	1.06	9.28
Khutala	3.4	33.0	21.1	42.5	51.25	2.68	1.21	0.99	7.47
Kleinkopje	2.8	15.4	24.0	57.8	68.88	3.77	1.54	0.69	6.92
Koornfontein	2.8	13.2	26.3	57.7	70.36	4.07	1.55	0.63	7.39
Kriel	4.6	26.8	22.9	45.8	54.5	2.9	1.3	0.8	9.2
Lakeside	4.4	11.6	26.0	58.0	69.44	3.62	1.66	0.38	8.90
Landau (Kromdraai)	2.8	14.2	23.8	59.2	69.34	3.95	1.55	0.59	7.57
Leeuwfontein	4.4	12.7	26.7	56.3	68.8	3.7	1.5	0.4	8.6
Leeuwpan	2.9	14.1	24.6	58.4	68.53	3.59	1.59	0.64	8.65
Leeuwspruit	2.6	13.8	28.8	54.8	70.83	4.03	1.62	0.81	6.31
Lemoenfontein	3.8	8.3	33.6	54.3	72.80	4.58	1.72	1.65	7.15
Matla	5.3	27.1	24.1	43.5	52.71	2.91	1.29	1.08	9.61
Middelburg Consolidated	2.5	14.1	24.2	59.2	70.25	3.77	1.57	0.45	7.37
New Clydesdale	2.6	6.8	31.2	59.4	75.99	4.59	1.74	0.57	7.71
New Denmark	3.5	31.6	21.9	43.0	52.08	2.80	1.40	1.25	7.37
Olifantslaagte	5.0	13.4	24.0	57.6	67.16	3.71	1.58	0.24	8.91
Optimum	3.4	16.7	27.9	52.0	66.1	3.8	1.5	0.6	7.8
Phoenix	2.7	15.8	26.6	54.9	69.06	3.63	1.35	0.30	7.16
Polmaise	3.0	11.2	25.9	59.9	72.78	4.06	1.81	0.54	6.61
Rietspruit	3.1	13.8	26.9	56.2	69.74	4.05	1.58	0.65	7.08
Secunda: Bosjesspruit	3.9	32.8	21.6	41.7	50.48	2.74	1.23	1.61	7.24
Secunda: Middelbult	4.2	23.8	22.7	49.3	58.31	2.98	1.44	1.12	8.15
Secunda: Brandspruit	4.4	23.8	22.6	49.2	56.25	2.87	1.52	1.04	10.12
Secunda: Syferfontein	5.6	28.3	22.0	44.1	52.18	2.75	1.30	0.75	9.12
Secunda: Twistdraai	3.7	23.3	27.2	45.9	58.6	3.5	1.5	1.1	8.4
South Witbank	3.7	16.0	28.2	52.1	66.61	3.77	1.58	0.96	7.38
Leeuwpan (Stuart)	3.2	20.1	29.1	47.6	62.72	3.95	1.47	0.49	8.07
Tavistock: No. 4 Seam	3.4	11.3	27.3	58.0	71.43	3.89	1.70	0.66	7.62
Van Dyks Drift	2.5	12.3	26.9	58.4	72.0	4.2	1.6	0.6	6.9
Waterpan	3.4	11.6	27.4	57.6	72.00	3.72	1.78	0.57	6.93
Witbank	3.2	14.1	25.7	57.1	69.6	3.6	1.6	0.7	7.2
Woestalleen	4.0	12.1	25.6	58.3	70.35	3.74	1.67	0.64	7.50

COLLIERY	PROXIMATE ANALYSIS				ULTIMATE ANALYSIS				
	Moisture	Ash	Volatile matter	Fixed carbon	C	H	N	S	O
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Belfast - Carolina - Ermelo									
Bituminous									
Coastal Fuels: Paardeplaats	2.9	10.6	36.2	50.3	71.17	4.70	1.74	1.09	7.80
Coastal Fuels: Witkrans	2.5	17.1	29.7	50.7	66.34	4.14	1.60	0.57	7.75
Delta	2.9	13.5	28.2	55.4	69.52	4.05	1.82	0.90	7.31
Eastside	2.8	8.7	33.2	55.3	73.90	4.70	1.88	0.69	7.33
Glisa	4.1	18.6	22.8	54.5	62.46	3.20	1.46	0.85	9.33
Golfview	3.7	15.1	30.2	51.1	66.1	4.0	1.9	0.8	8.5
Spitzkop	3.1	14.0	30.4	52.6	68.8	4.2	1.7	1.2	7.1
Strathrae	4.0	14.3	24.2	57.5	67.99	3.46	1.61	0.65	7.99
Sumo	5.4	13.1	22.8	58.7	68.52	3.36	1.58	0.33	7.71
Tselentis (Bothasrust)	3.2	14.7	26.5	55.6	69.39	3.86	1.48	0.56	6.81
Piet Retief - Wakkerstroom									
Anthracitic									
Protea	3.2	18.4	6.0	72.4	73.92	2.07	1.31	0.68	0.42
Bituminous									
Savmore	3.7	12.8	28.5	55.0	69.70	3.69	1.87	1.40	6.84
TBS	4.4	14.2	32.6	48.8	65.89	4.27	1.73	0.98	8.53
Kangwane (Komatipoort)									
Anthracitic									
Nkomati Anthracite	1.5	14.7	7.8	76.0	78.40	2.58	1.62	0.35	0.85
NORTHERN PROVINCE									
Ellisras									
Bituminous									
Grootegeluk	2.9	19.8	28.6	48.7	63.8	4.0	1.2	1.0	7.3
Venda									
Bituminous									
Tshikondeni	0.8	12.5	23.7	63.0	78.41	4.23	1.60	0.94	1.53
FREE STATE									
Sasolburg									
Bituminous									
New Vaal	5.9	40.2	22.3	31.6	40.90	2.43	0.95	0.55	9.07
Sigma	6.2	31.5	21.9	40.4	49.73	2.50	1.21	0.93	7.93
KWAZULU-NATAL									
Dundee - Newcastle - Utrecht									
Anthracitic									
CBR Mining	2.0	12.8	10.9	74.3	75.79	3.13	2.04	1.34	2.90
Springlake	1.7	12.3	10.3	75.7	77.80	3.25	2.06	1.55	1.34
Bituminous									
CBR Mining	1.9	17.0	16.5	64.6	71.40	3.37	1.92	1.60	2.81
Durban Navigation	1.5	11.5	30.1	56.9	74.69	4.75	2.00	1.46	4.10
Welgedacht	3.1	13.9	28.0	55.0	69.76	4.03	1.81	1.53	5.87
Vryheid									
Anthracitic									
Duiker: Dixon (Gus)	3.3	12.0	5.2	79.5	78.93	2.15	1.64	0.90	1.08
Duiker: Enyati (Alfred)	3.0	13.9	5.4	77.7	77.44	2.05	1.77	0.89	0.95
Duiker: Oakhurst	2.1	12.5	9.8	75.6	78.90	3.03	2.23	0.74	0.50
Duiker: Dundas Seam	2.8	16.3	7.4	73.5	73.90	2.53	1.77	0.53	2.17
Rietvlei	4.1	11.8	5.5	78.6	78.32	2.35	1.89	1.25	0.29
Bituminous									
Recmin	3.9	24.8	13.0	58.3	61.85	2.90	1.75	0.69	4.11
Vryheid Coronation	1.0	12.0	20.2	66.8	79.05	3.98	1.86	0.70	1.41
Ulundi									
Anthracitic									
Zululand Anthracite	2.9	16.4	6.9	73.9	75.0	2.3	1.6	1.2	0.7
SWAZILAND									
Anthracitic									
Maloma	1.8	9.9	6.1	82.2	82.04	2.89	1.94	0.64	0.79

Table C-4: Proximate and ultimate analysis data (per province)

Province	PROXIMATE ANALYSIS				ULTIMATE ANALYSIS				
	Moisture	Ash	Volatile matter	Fixed carbon	C	H	N	S	O
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
MPUMALANGA									
Bituminous	3.4	16.0	26.6	54.0	66.9	3.8	1.6	0.7	7.6
Anthracitic	2.4	16.6	6.9	74.2	76.2	2.3	1.5	0.5	0.6
NORTHERN PROVINCE									
Bituminous	2.4	18.0	27.4	52.3	67.4	4.1	1.3	1.0	5.9
FREE STATE									
Bituminous	6.1	35.9	22.1	36.0	45.3	2.5	1.1	0.7	8.5
KWAZULU-NATAL									
Bituminous	2.3	15.8	21.6	60.3	71.4	3.8	1.9	1.2	3.7
Anthracitic	2.8	13.8	7.6	75.8	76.8	2.6	1.8	1.1	1.2
SWAZILAND									
Anthracitic	1.8	9.9	6.1	82.2	82.04	2.89	1.94	0.64	0.79

Table C-5: Proximate and ultimate analysis data (per coal type)

Coal type	PROXIMATE ANALYSIS				ULTIMATE ANALYSIS				
	Moisture	Ash	Volatile matter	Fixed carbon	C	H	N	S	O
	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)	(%)
Bituminous	3.3	16.4	26.3	54.0	66.8	3.8	1.6	0.8	7.4
Anthracitic	2.6	14.0	7.3	76.1	77.1	2.6	1.8	0.9	1.1

Table C-6: Moisture elemental analysis

Element	*Molar mass (g/mol)*	*Elemental mass% composition*
H	1.01	**11.2%**
O	16	**88.8%**
H_2O	18.02	**100.0%**

D. APPENDIX D: Case studies - Additional furnaces (Chapter 2)

Table D-1: Results for additional case studies - Chapter 2 (furnace 1-16)

Furnace	Case study	*CO_2 emissions (tonnes)*	*Error (%)*	Furnace	Case study	*CO_2 emissions (tonnes)*	*Error (%)*
1	**CS1**	108 486	18.8%	**9**	**CS1**	112 120	18.8%
	CS2	104 678	13.4%		**CS2**	119 072	14.6%
	CS3	114 188	8.0%		**CS3**	128 809	7.1%
2	**CS1**	139 820	18.8%	**10**	**CS1**	111 377	18.8%
	CS2	132 592	13.5%		**CS2**	117 198	14.5%
	CS3	144 637	8.0%		**CS3**	126 815	7.2%
3	**CS1**	192 005	18.8%	**11**	**CS1**	54 670	18.8%
	CS2	112 139	1.1%		**CS2**	57 946	14.4%
	CS3	129 486	14.1%		**CS3**	63 053	7.4%
4	**CS1**	238 526	18.8%	**12**	**CS1**	76 435	18.8%
	CS2	141 055	2.5%		**CS2**	74 808	15.9%
	CS3	161 294	13.7%		**CS3**	81 289	7.0%
5	**CS1**	70 557	18.8%	**13**	**CS1**	185 983	18.8%
	CS2	77 353	13.1%		**CS2**	139 605	9.8%
	CS3	83 956	7.7%		**CS3**	152 137	9.7%
6	**CS1**	95 753	18.8%	**14**	**CS1**	203 825	18.8%
	CS2	103 456	12.2%		**CS2**	159 129	9.4%
	CS3	112 565	8.0%		**CS3**	173 753	9.7%
7	**CS1**	78 482	18.8%	**15**	**CS1**	171 811	18.8%
	CS2	85 030	12.3%		**CS2**	162 664	13.7%
	CS3	92 456	8.0%		**CS3**	176 802	7.8%
8	**CS1**	104 255	18.8%	**16**	**CS1**	148 527	18.8%
	CS2	112 102	12.0%		**CS2**	126 658	7.9%
	CS3	121 925	8.1%		**CS3**	140 354	10.9%

Furnace 1:

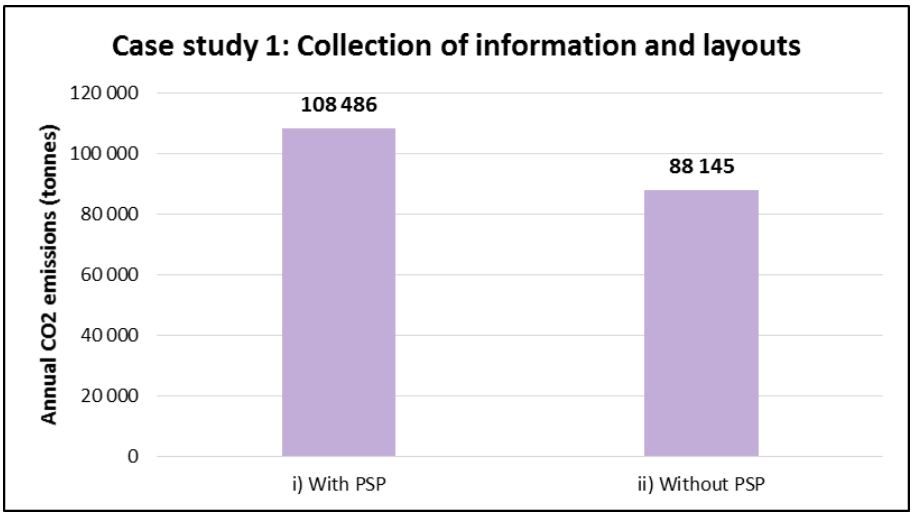


Figure D-1: Additional CS1 for Chapter 2 (Furnace 1)

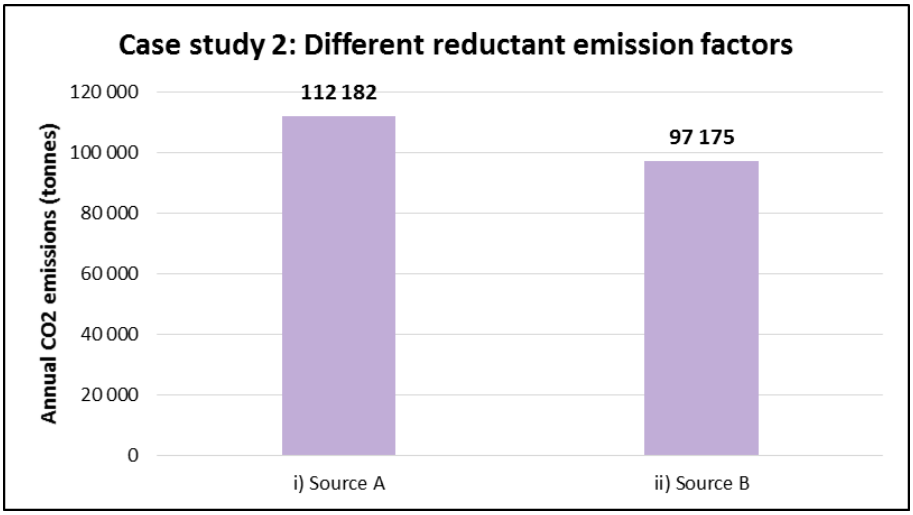


Figure D-2: Additional CS2 for Chapter 2 (Furnace 1)

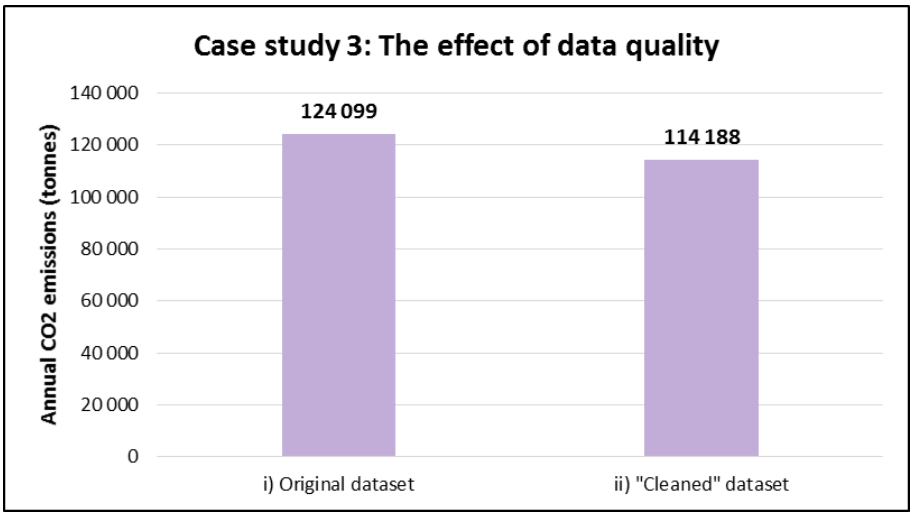


Figure D-3: Additional CS3 for Chapter 2 (Furnace 1)

Furnace 2:

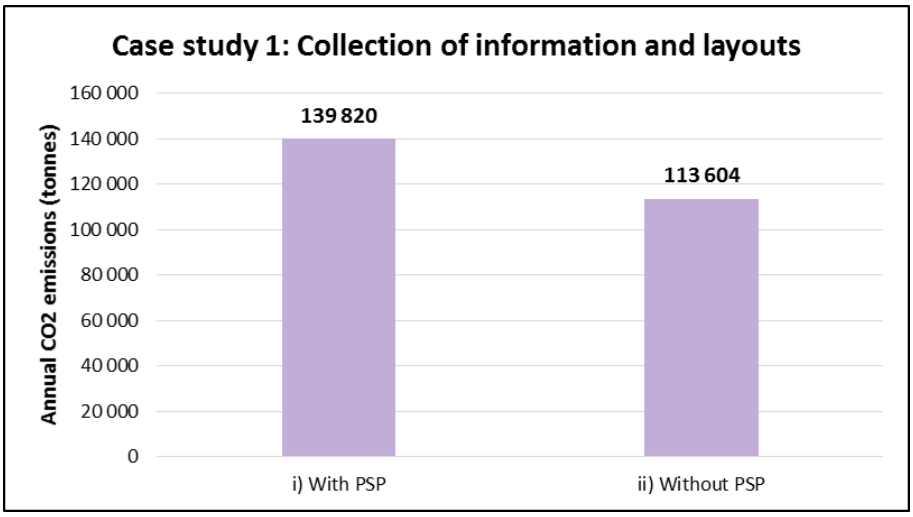


Figure D-4: Additional CS1 for Chapter 2 (Furnace 2)

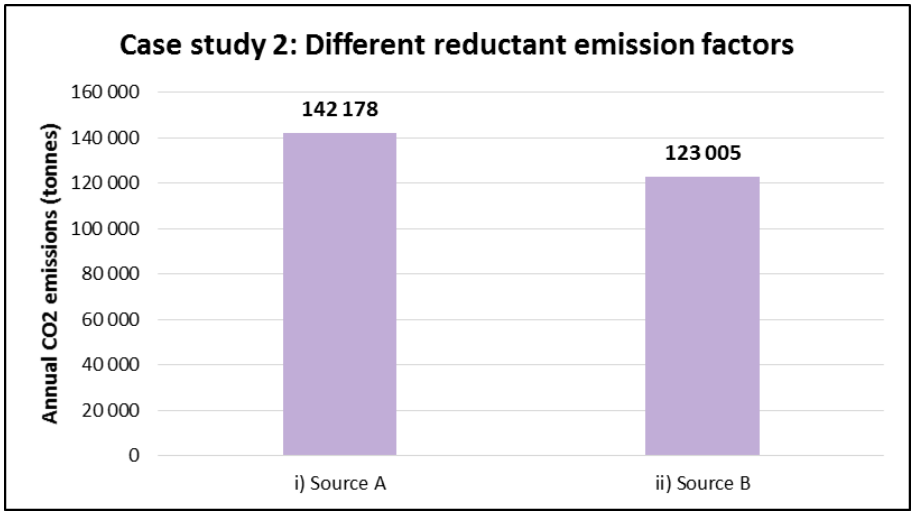


Figure D-5: Additional CS2 for Chapter 2 (Furnace 2)

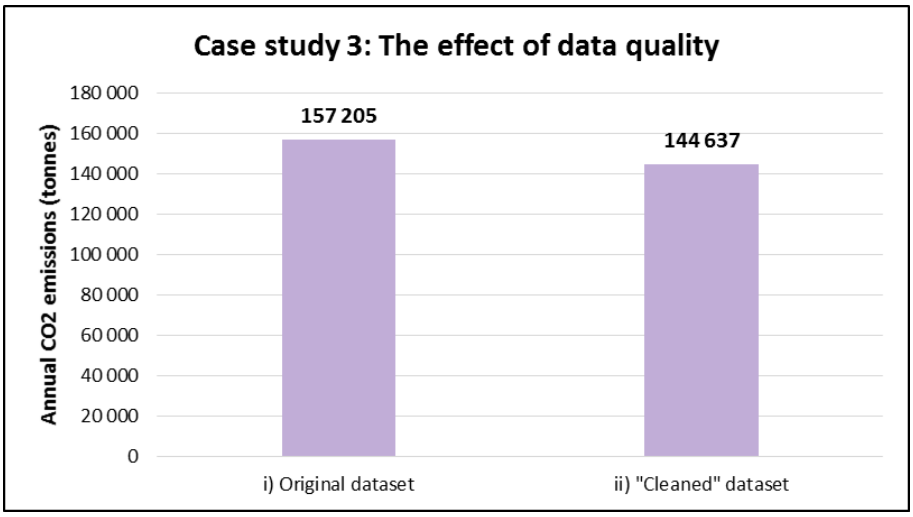


Figure D-6: Additional CS3 for Chapter 2 (Furnace 2)

Furnace 3:

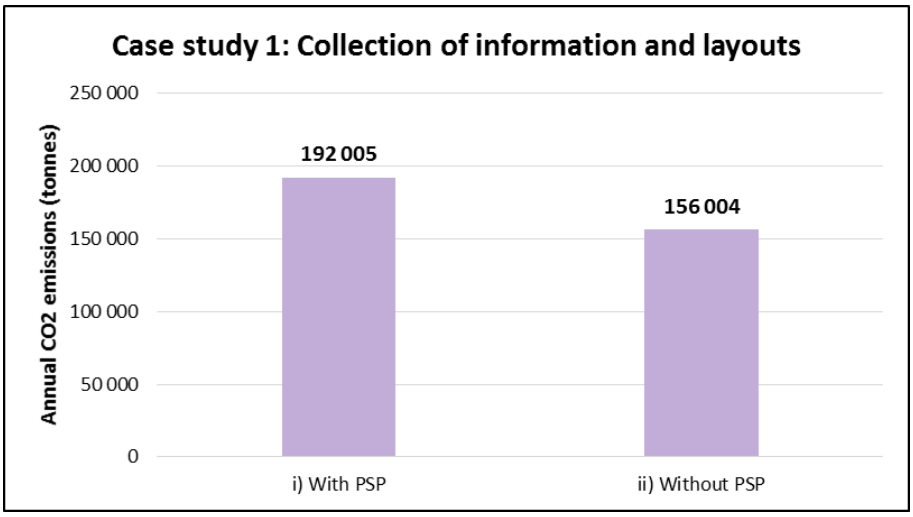


Figure D-7: Additional CS1 for Chapter 2 (Furnace 3)

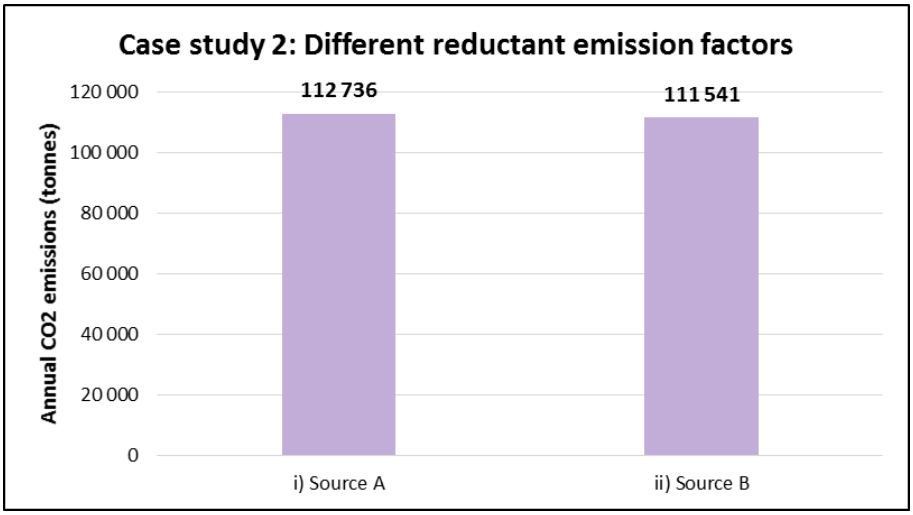


Figure D-8: Additional CS2 for Chapter 2 (Furnace 3)

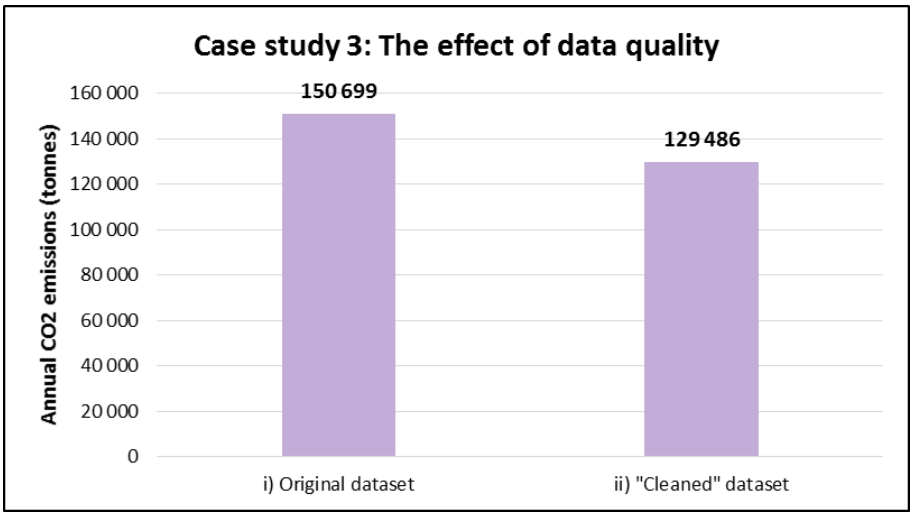


Figure D-9: Additional CS3 for Chapter 2 (Furnace 3)

Furnace 4:

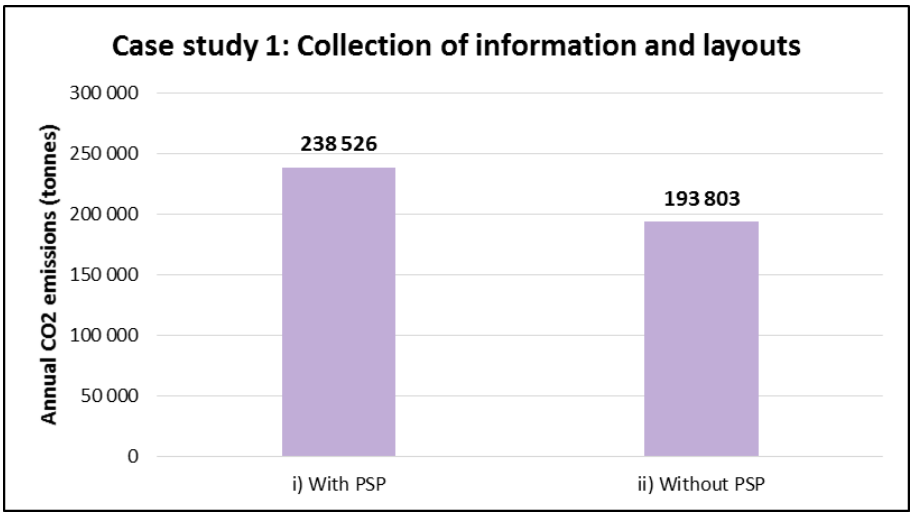


Figure D-10: Additional CS1 for Chapter 2 (Furnace 4)

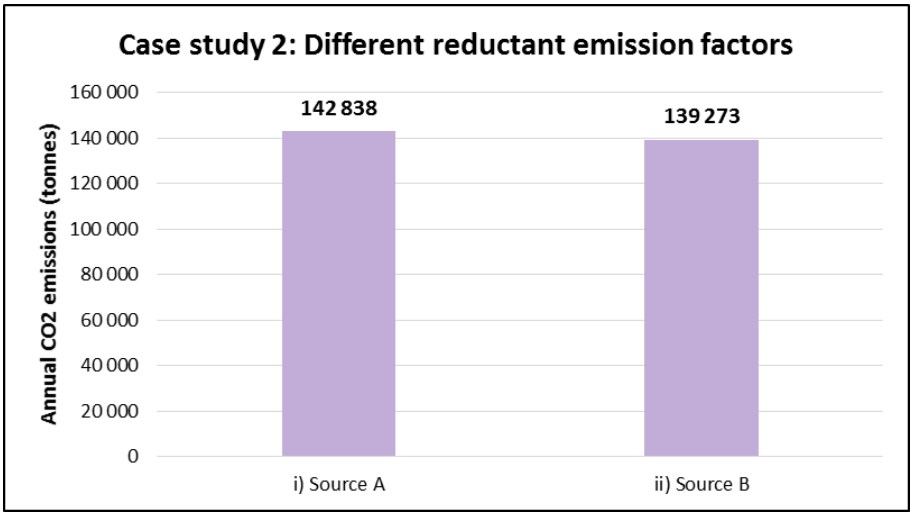


Figure D-11: Additional CS2 for Chapter 2 (Furnace 4)

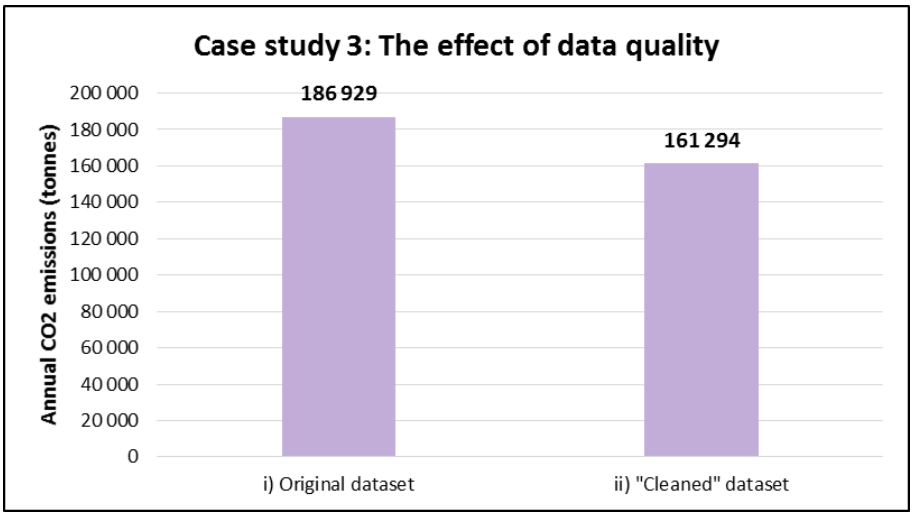


Figure D-12: Additional CS3 for Chapter 2 (Furnace 4)

Furnace 5:

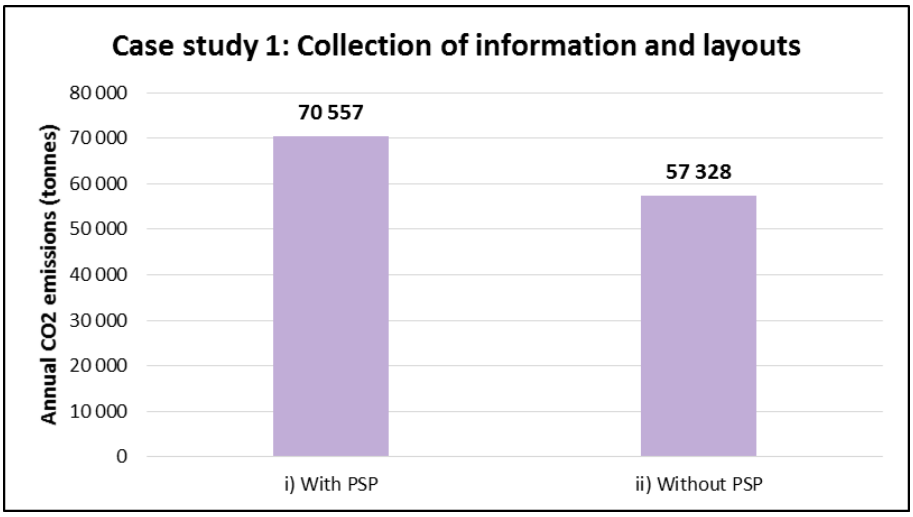


Figure D-13: Additional CS1 for Chapter 2 (Furnace 5)

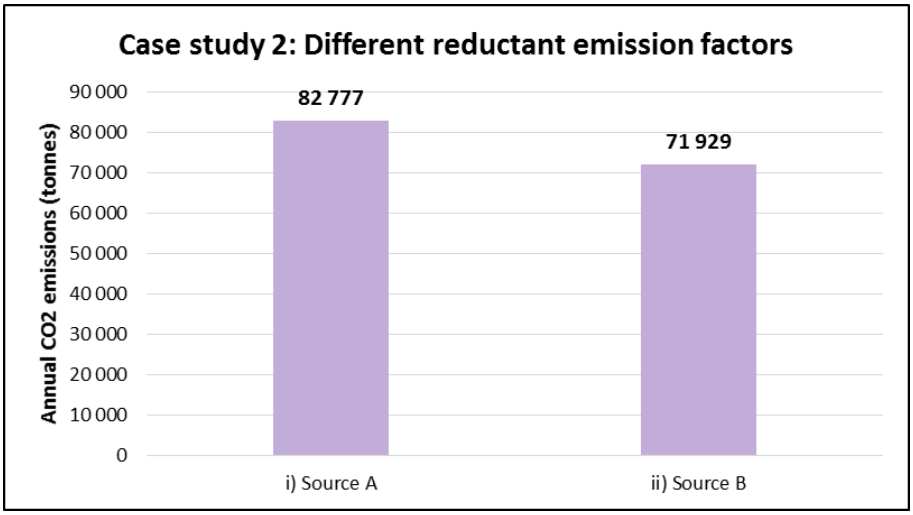


Figure D-14: Additional CS2 for Chapter 2 (Furnace 5)

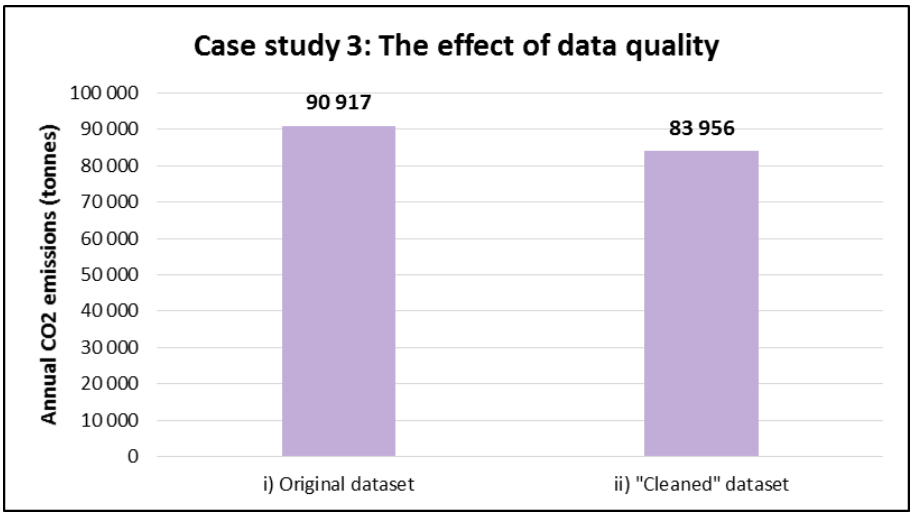


Figure D-15: Additional CS3 for Chapter 2 (Furnace 5)

Furnace 6:

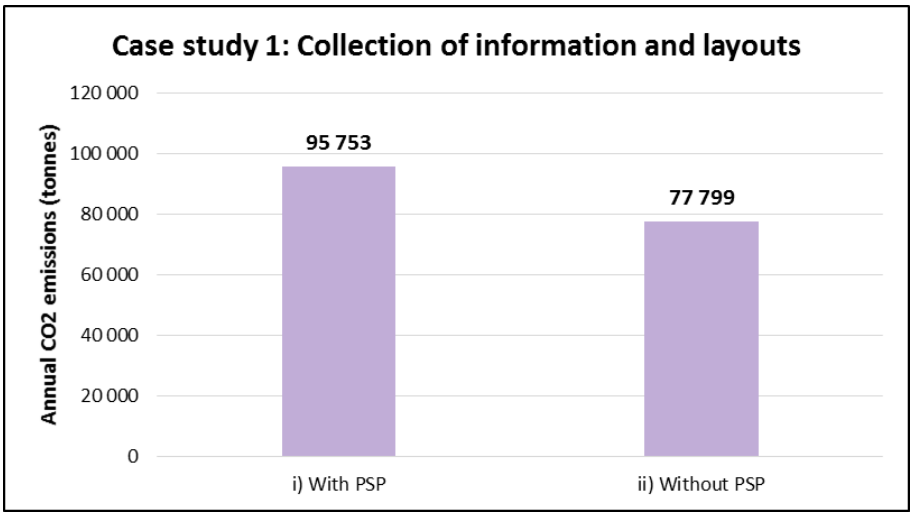


Figure D-16: Additional CS1 for Chapter 2 (Furnace 6)

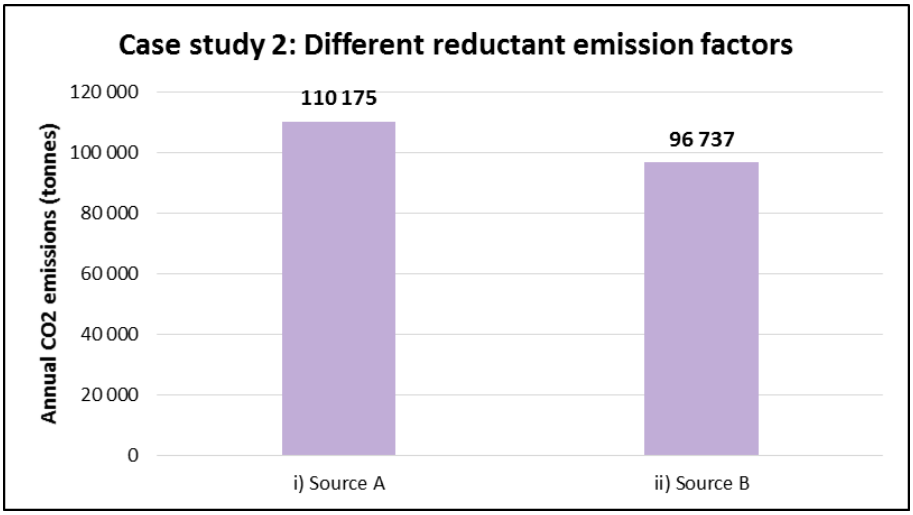


Figure D-17: Additional CS2 for Chapter 2 (Furnace 6)

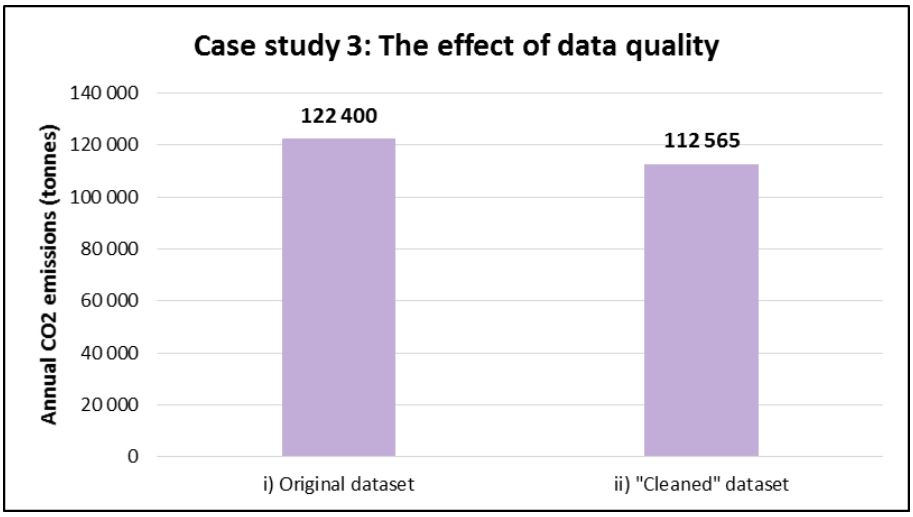


Figure D-18: Additional CS3 for Chapter 2 (Furnace 6)

Furnace 7:

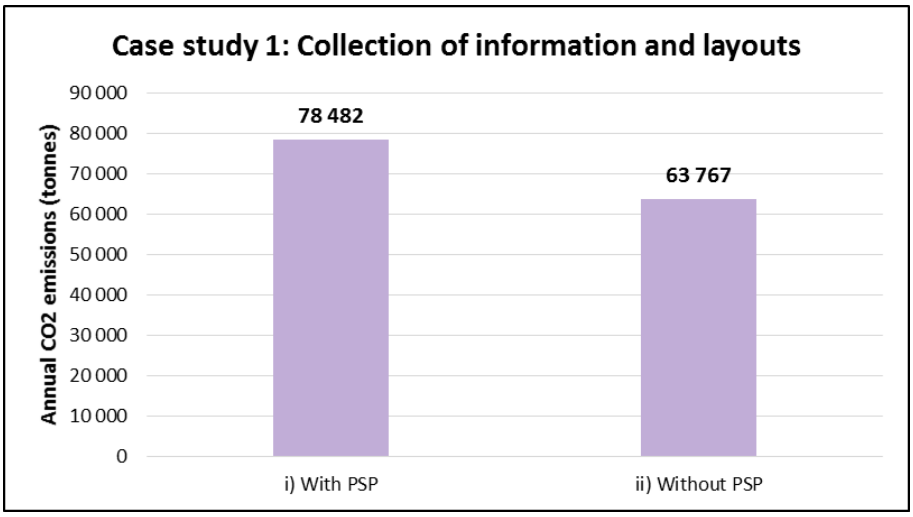


Figure D-19: Additional CS1 for Chapter 2 (Furnace 7)

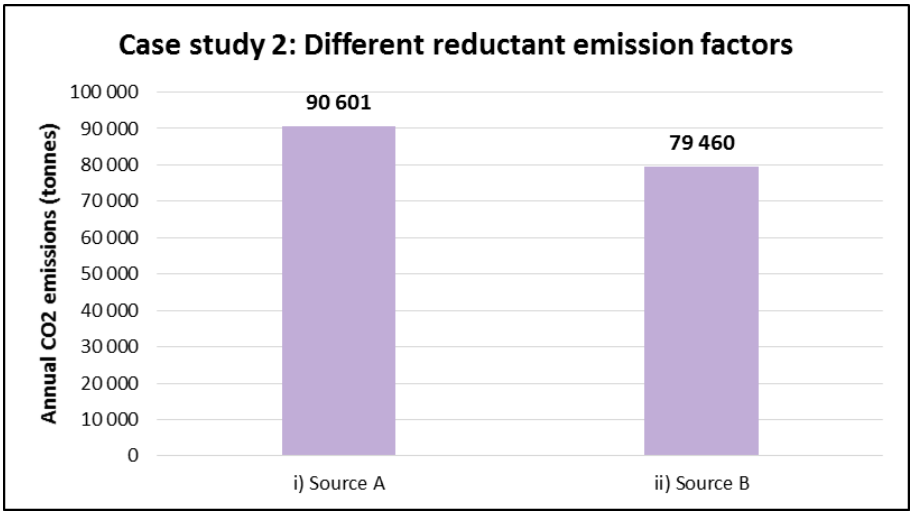


Figure D-20: Additional CS2 for Chapter 2 (Furnace 7)

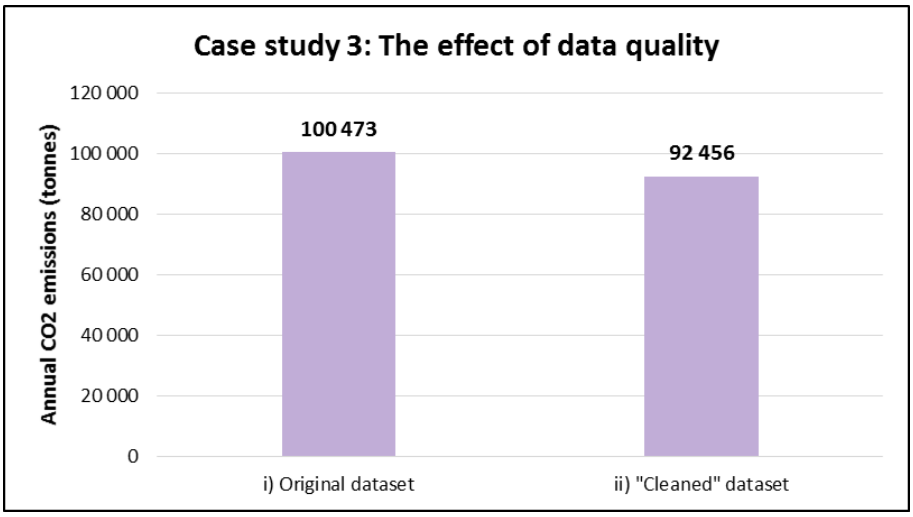


Figure D-21: Additional CS3 for Chapter 2 (Furnace 7)

Furnace 8:

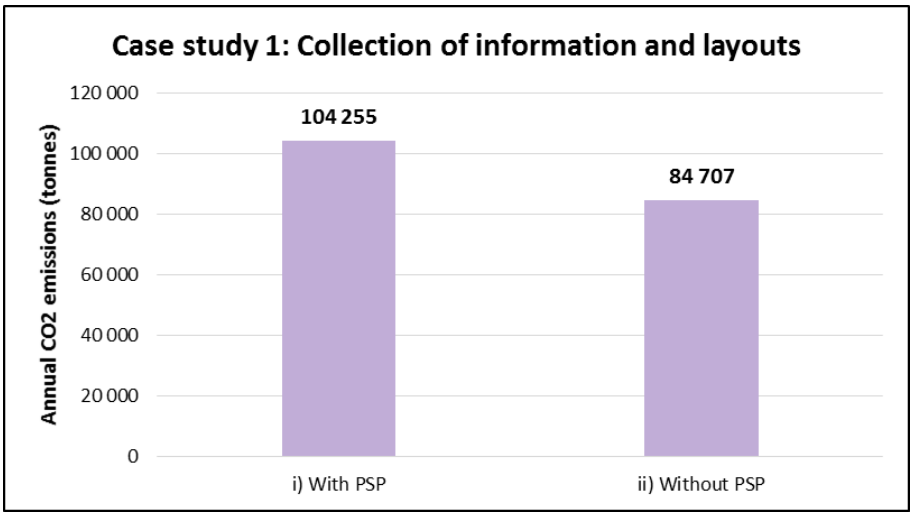


Figure D-22: Additional CS1 for Chapter 2 (Furnace 8)

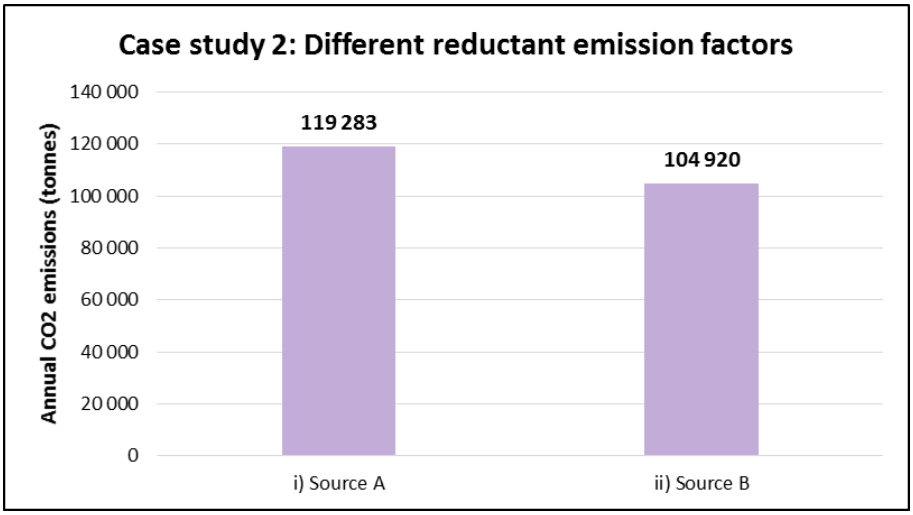


Figure D-23: Additional CS2 for Chapter 2 (Furnace 8)

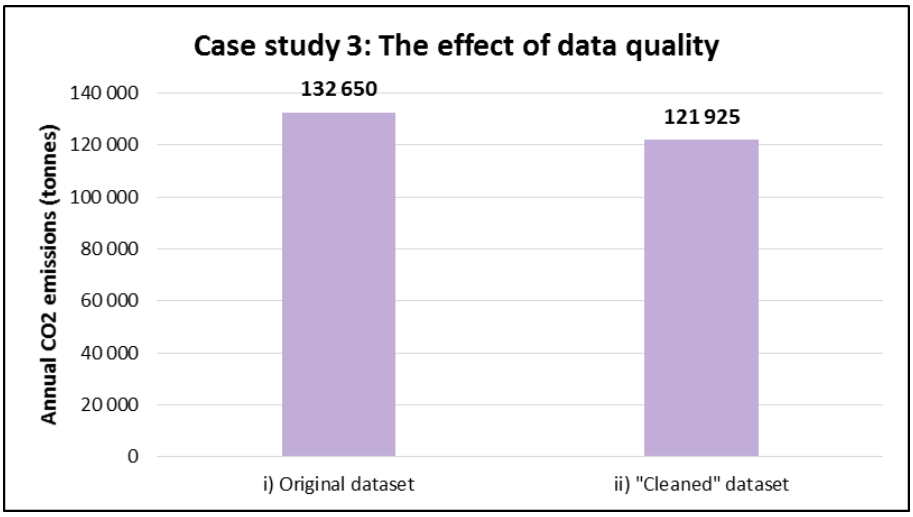


Figure D-24: Additional CS3 for Chapter 2 (Furnace 8)

Furnace 9:

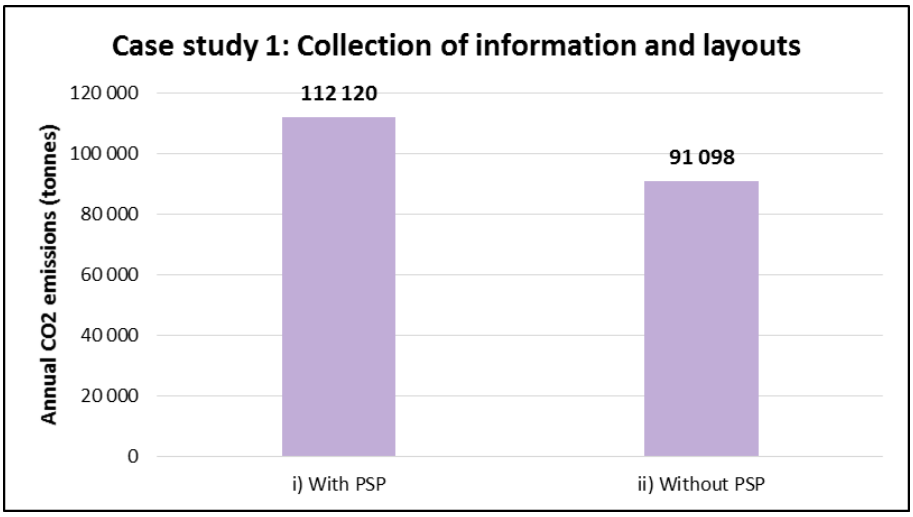


Figure D-25: Additional CS1 for Chapter 2 (Furnace 9)

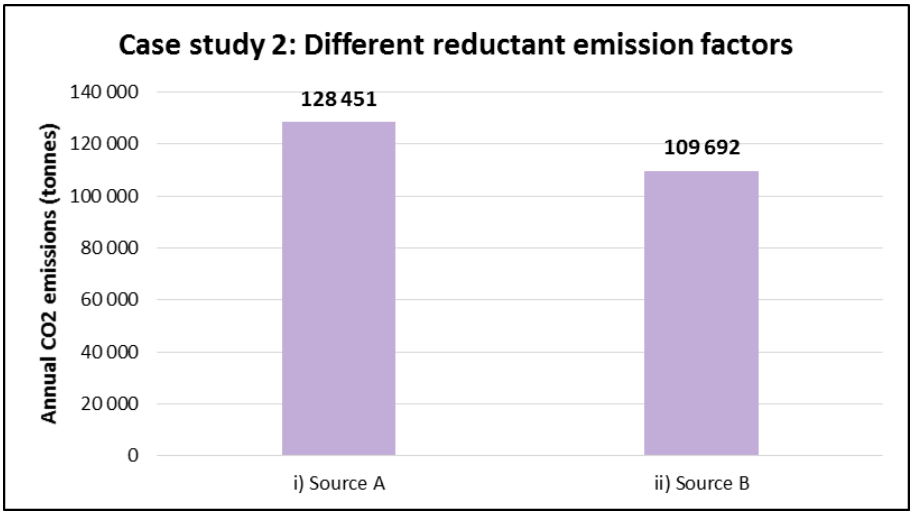


Figure D-26: Additional CS2 for Chapter 2 (Furnace 9)

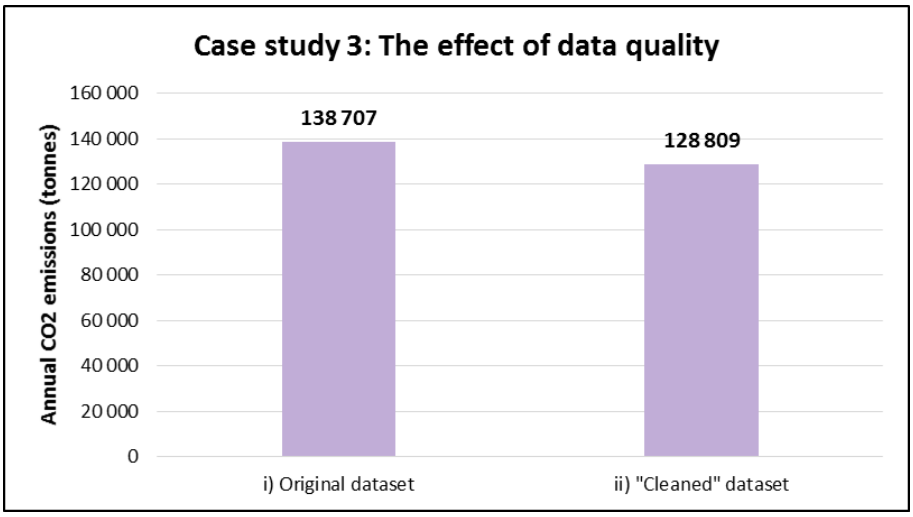


Figure D-27: Additional CS3 for Chapter 2 (Furnace 9)

Furnace 10:

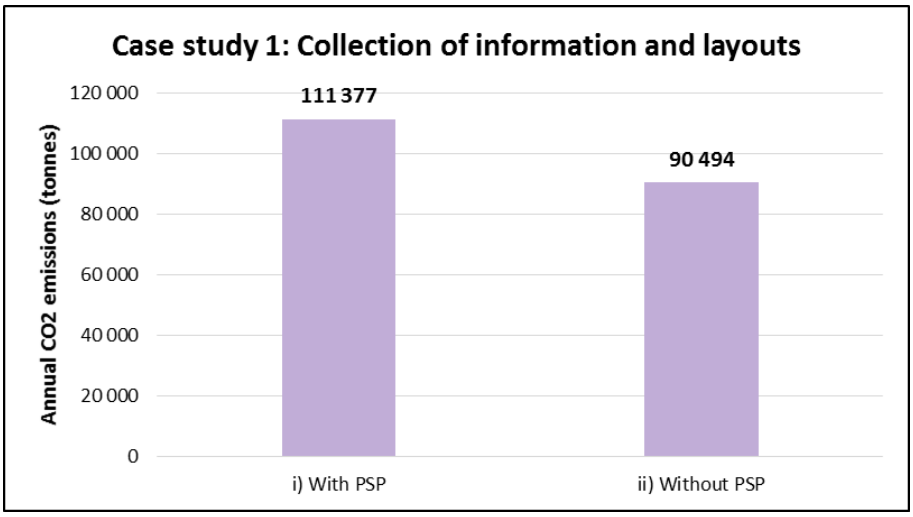


Figure D-28: Additional CS1 for Chapter 2 (Furnace 10)

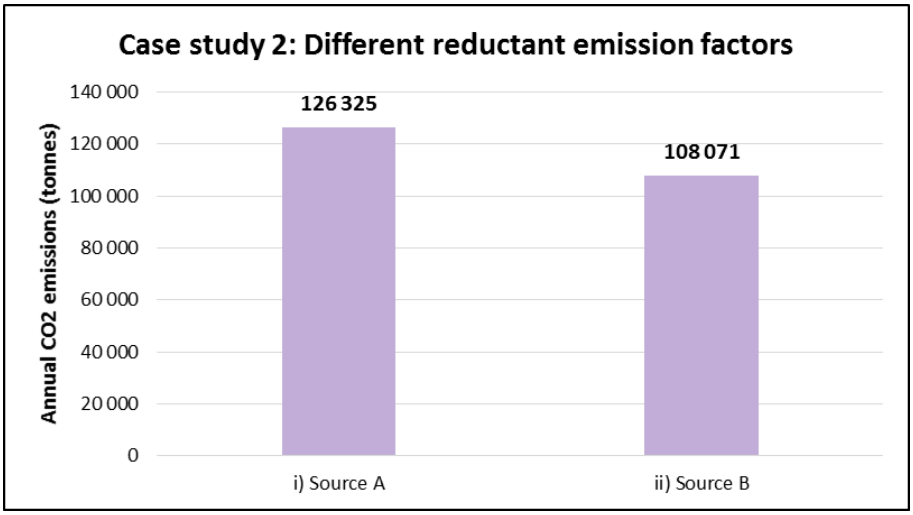


Figure D-29: Additional CS2 for Chapter 2 (Furnace 10)

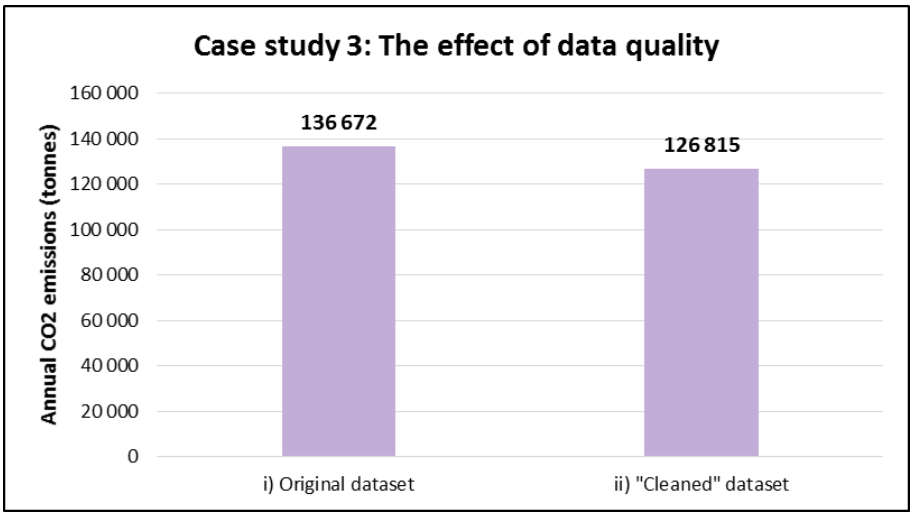


Figure D-30: Additional CS3 for Chapter 2 (Furnace 10)

Furnace 11:

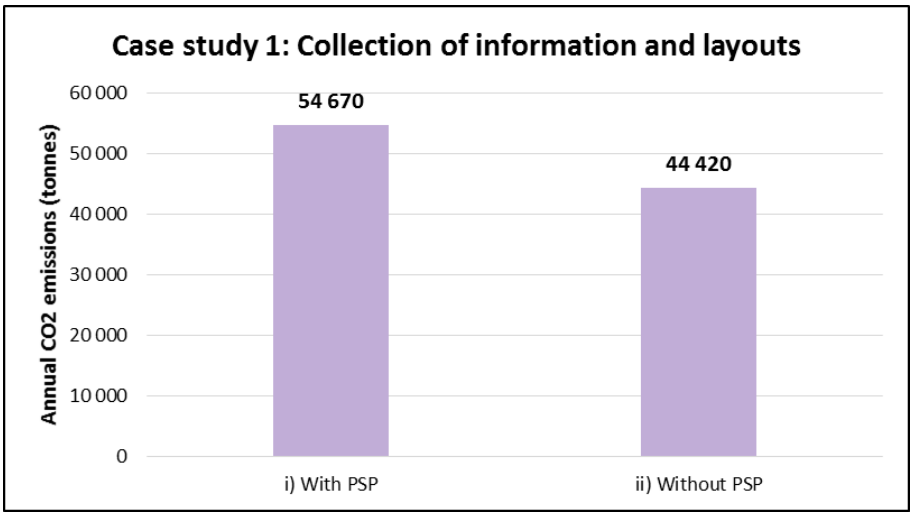


Figure D-31: Additional CS1 for Chapter 2 (Furnace 11)

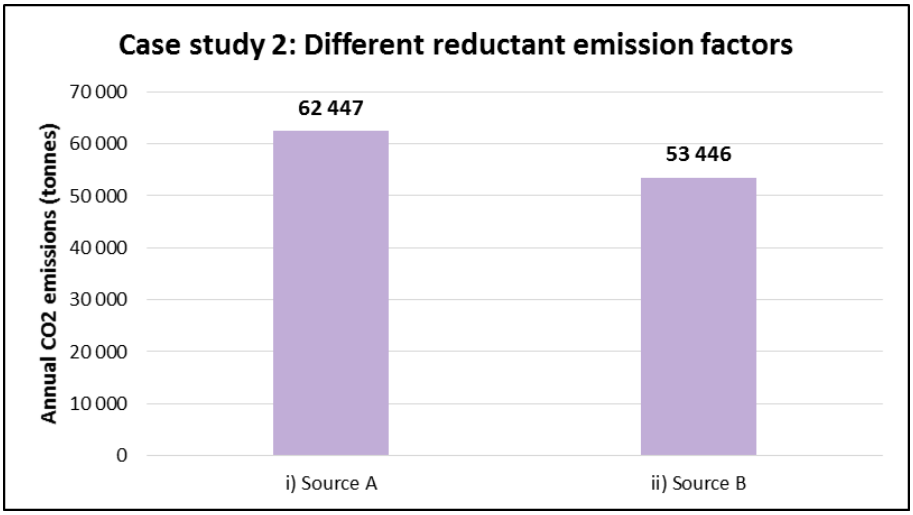


Figure D-32: Additional CS2 for Chapter 2 (Furnace 11)

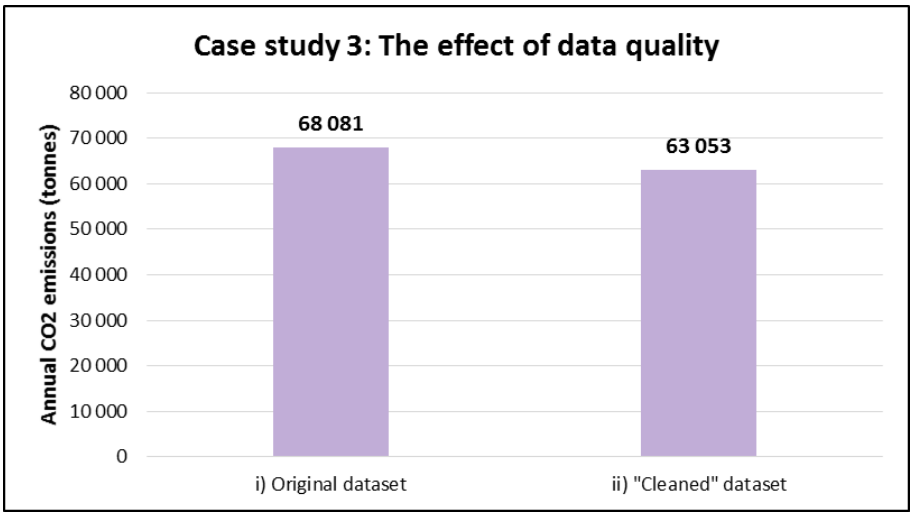


Figure D-33: Additional CS3 for Chapter 2 (Furnace 11)

Furnace 12:

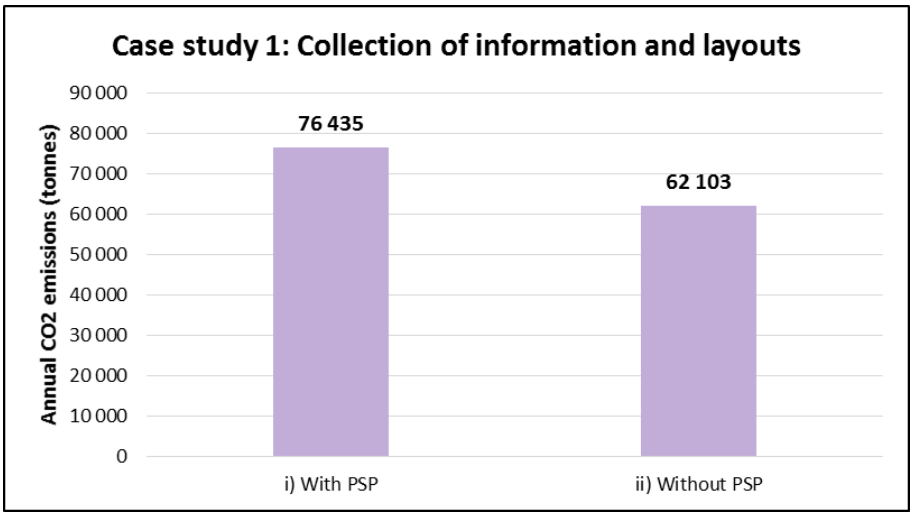


Figure D-34: Additional CS1 for Chapter 2 (Furnace 12)

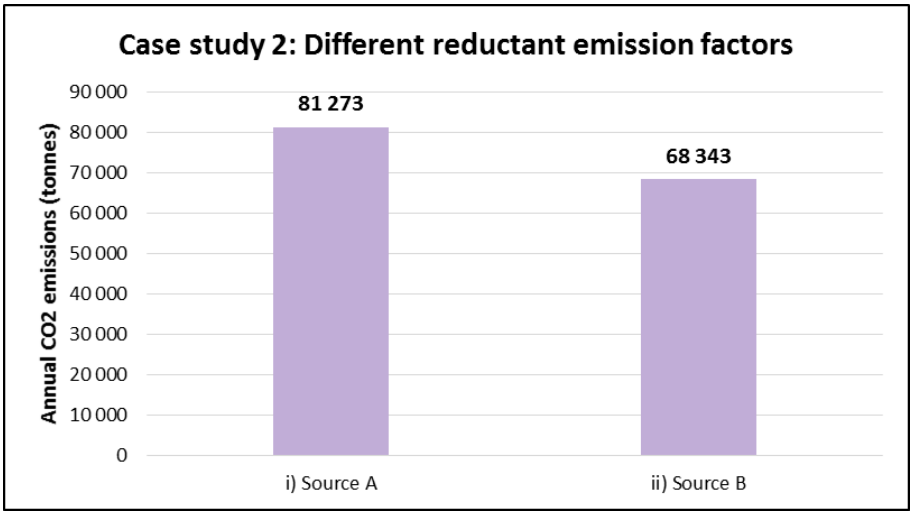


Figure D-35: Additional CS2 for Chapter 2 (Furnace 12)

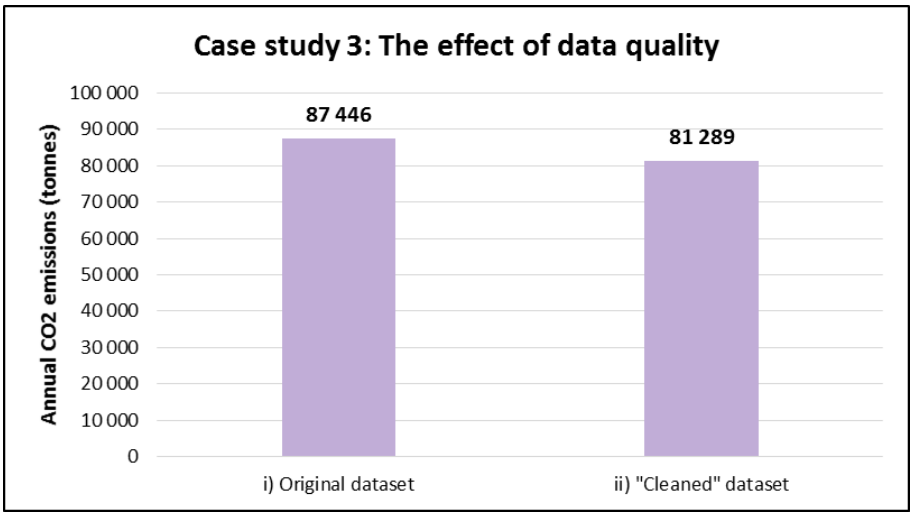


Figure D-36: Additional CS3 for Chapter 2 (Furnace 12)

Furnace 13:

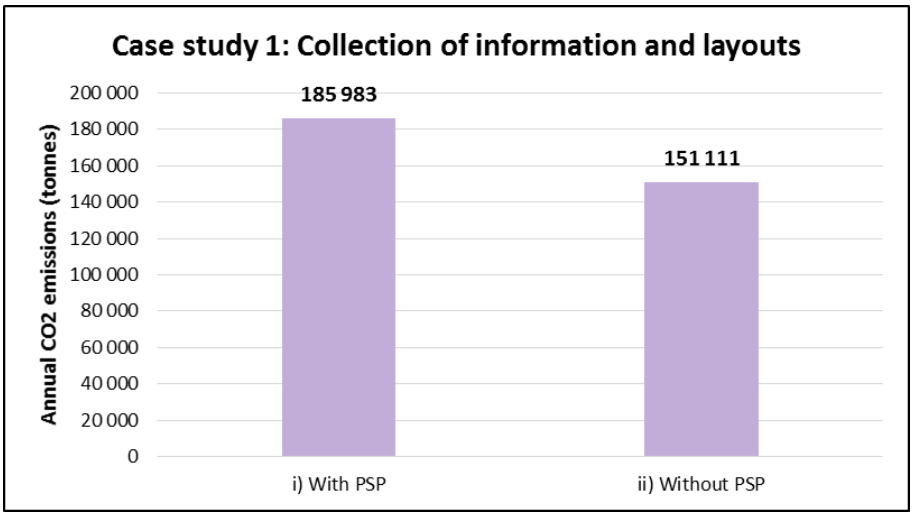


Figure D-37: Additional CS1 for Chapter 2 (Furnace 13)

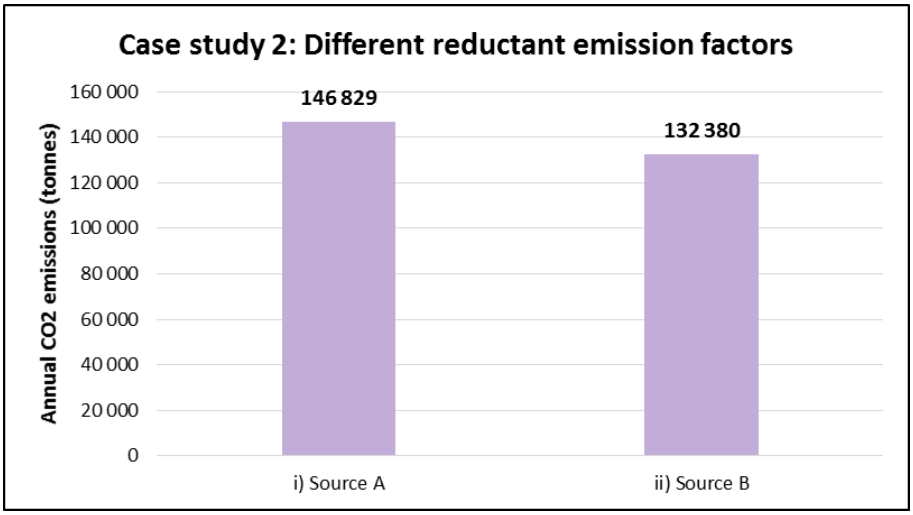


Figure D-38: Additional CS2 for Chapter 2 (Furnace 13)

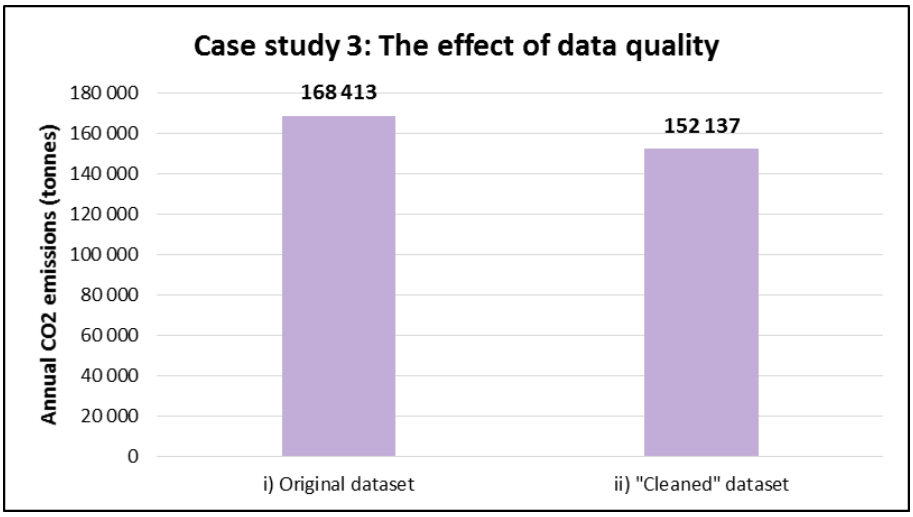


Figure D-39: Additional CS3 for Chapter 2 (Furnace 13)

Furnace 14:

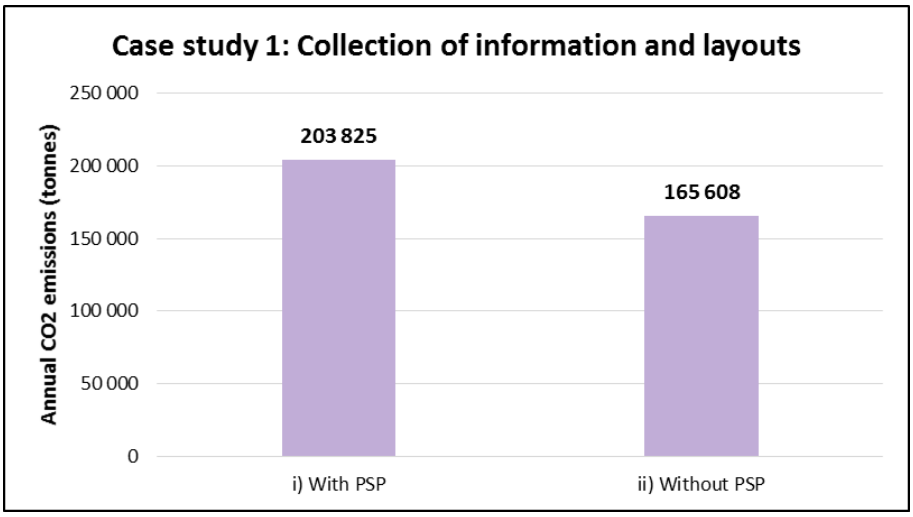


Figure D-40: Additional CS1 for Chapter 2 (Furnace 14)

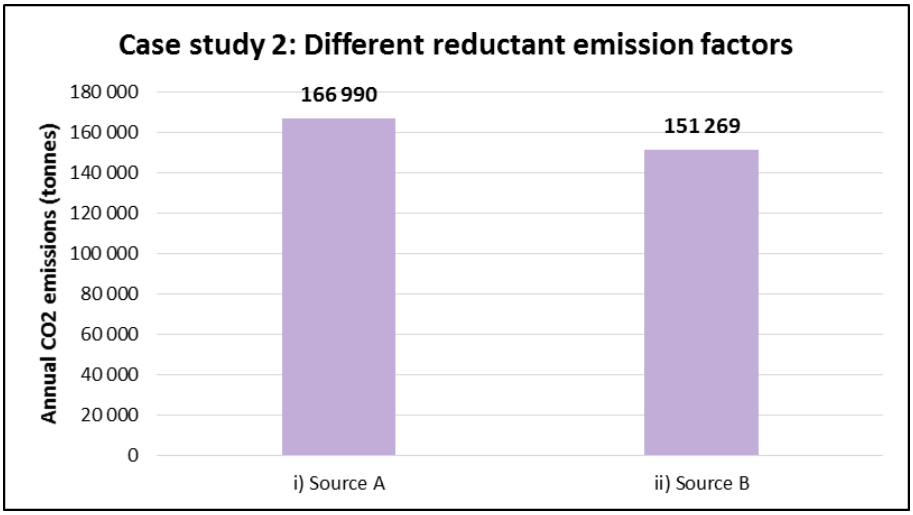


Figure D-41: Additional CS2 for Chapter 2 (Furnace 14)

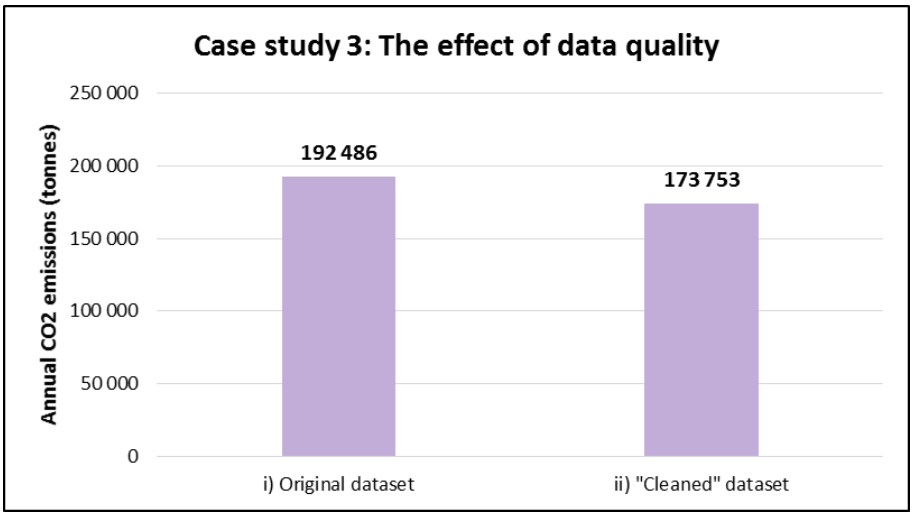


Figure D-42: Additional CS3 for Chapter 2 (Furnace 14)

Furnace 15:

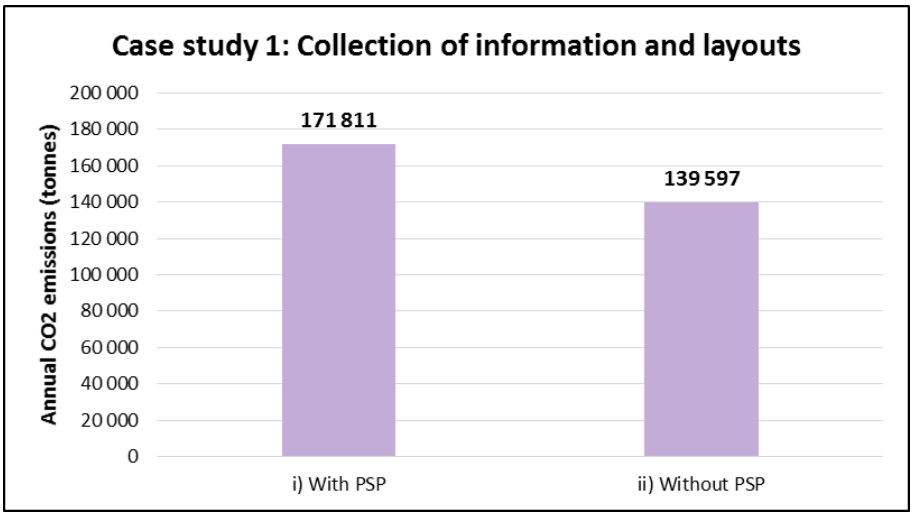


Figure D-43: Additional CS1 for Chapter 2 (Furnace 15)

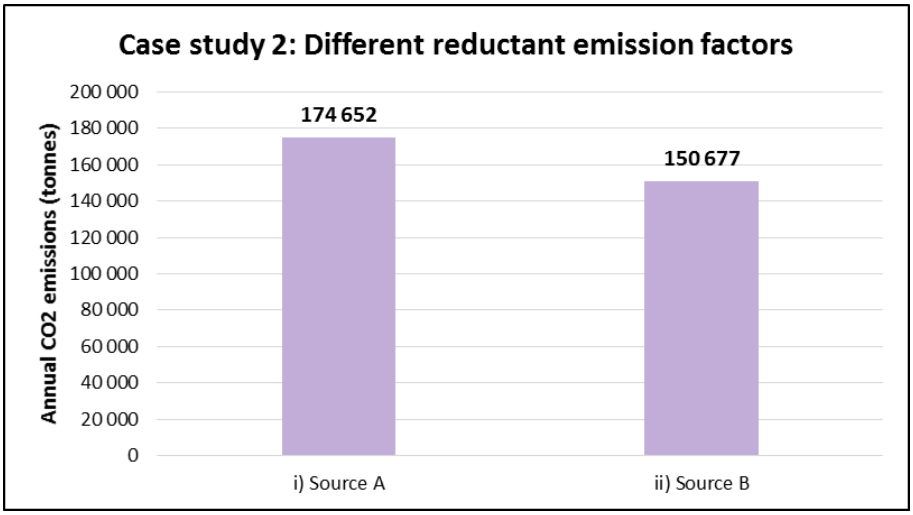


Figure D-44: Additional CS2 for Chapter 2 (Furnace 15)

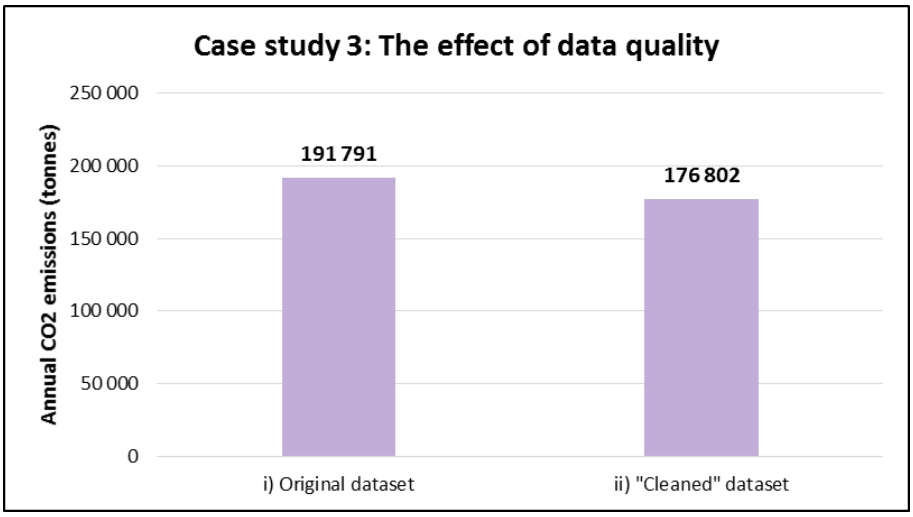


Figure D-45: Additional CS3 for Chapter 2 (Furnace 15)

Furnace 16:

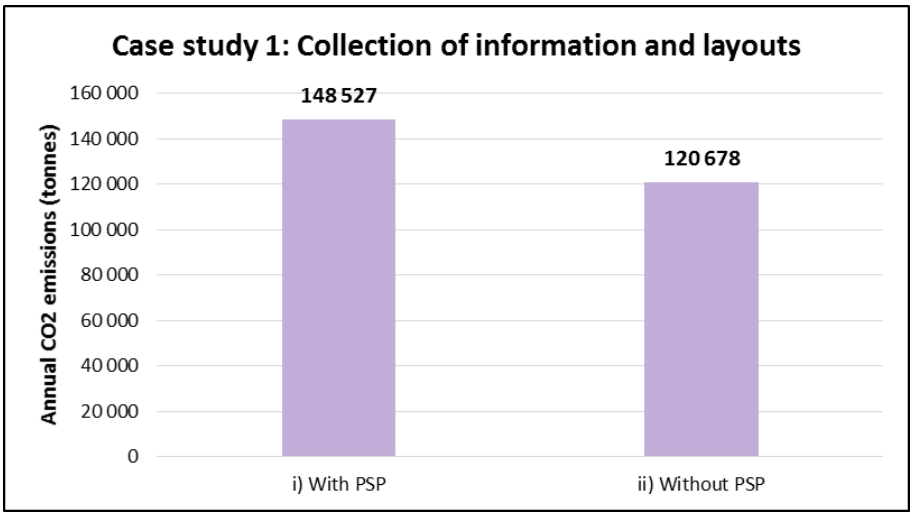


Figure D-46: Additional CS1 for Chapter 2 (Furnace 16)

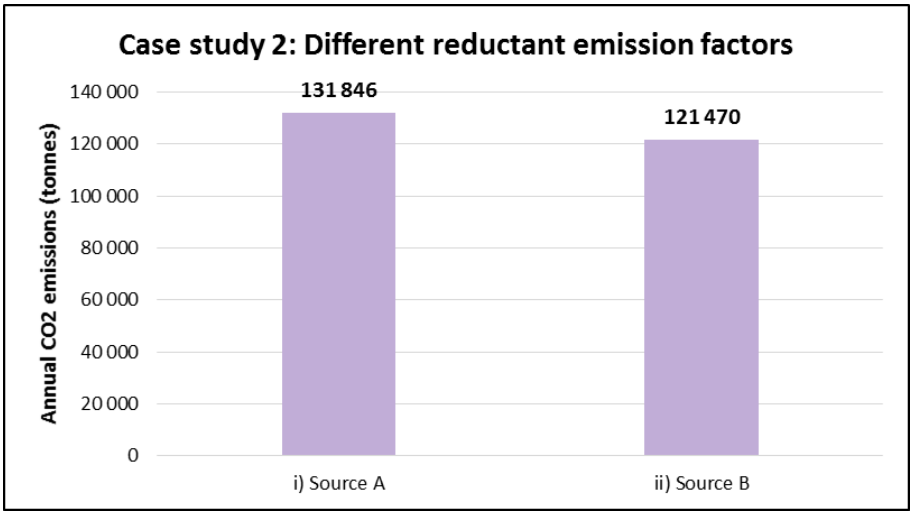


Figure D-47: Additional CS2 for Chapter 2 (Furnace 16)

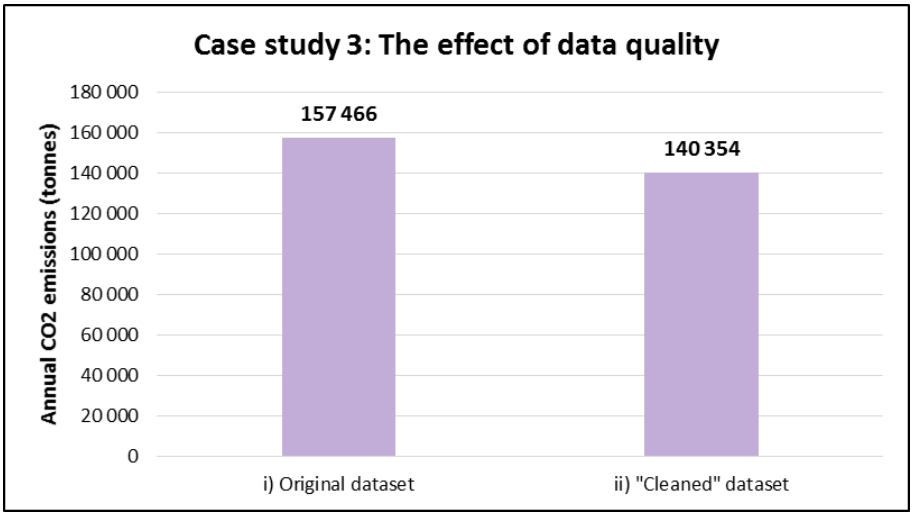


Figure D-48: Additional CS3 for Chapter 2 (Furnace 16)

E. APPENDIX E: Case studies – Additional furnaces (Chapter 3)

Table E-1: Results for additional case studies - Chapter 3 (furnace 1-16)

Furnace	Case study	*CO_2 emissions (tonnes)*	*Mass balance error (%)*	Furnace	Case study	*CO_2 emissions (tonnes)*	*Mass balance error (%)*
1	**CS1**	104 922	13.9%	**9**	**CS1**	95 906	16.1%
	CS2	96 249	15.3%		**CS2**	103 360	15.1%
	CS3	102 026	2.8%		**CS3**	116 302	2.4%
2	**CS1**	109 936	14.6%	**10**	**CS1**	86 726	16.5%
	CS2	122 215	12.9%		**CS2**	96 355	14.9%
	CS3	129 831	2.5%		**CS3**	114 777	1.7%
3	**CS1**	-24 595	56.4%	**11**	**CS1**	46 039	16.0%
	CS2	66 210	18.6%		**CS2**	53 905	15.3%
	CS3	101 381	8.3%		**CS3**	56 259	4.0%
4	**CS1**	-41 378	60.9%	**12**	**CS1**	49 183	17.0%
	CS2	75 439	21.3%		**CS2**	67 245	11.2%
	CS3	126 660	7.2%		**CS3**	72 693	1.5%
5	**CS1**	65 057	16.8%	**13**	**CS1**	74 632	21.4%
	CS2	71 222	16.2%		**CS2**	129 673	8.3%
	CS3	75 915	3.3%		**CS3**	140 060	1.0%
6	**CS1**	79 348	17.3%	**14**	**CS1**	95 409	19.4%
	CS2	86 891	16.3%		**CS2**	148 047	8.7%
	CS3	101 741	2.8%		**CS3**	160 321	0.9%
7	**CS1**	72 606	16.7%	**15**	**CS1**	110 059	16.3%
	CS2	78 105	16.4%		**CS2**	148 917	11.3%
	CS3	83 688	3.9%		**CS3**	160 329	1.6%
8	**CS1**	103 837	16.5%	**16**	**CS1**	81 471	16.7%
	CS2	106 975	15.9%		**CS2**	108 109	10.9%
	CS3	111 084	3.7%		**CS3**	121 648	2.1%

Furnace 1:

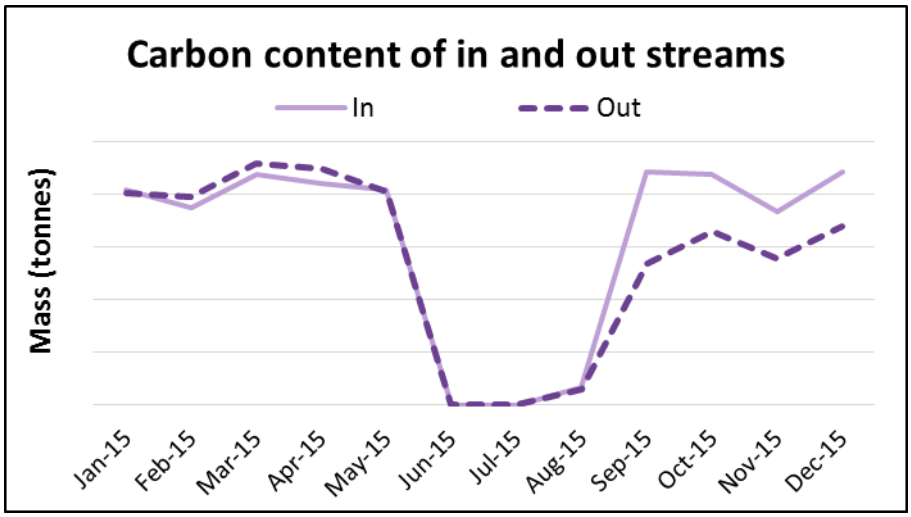


Figure E-1: Additional CS1 for Chapter 3 (Furnace 1)

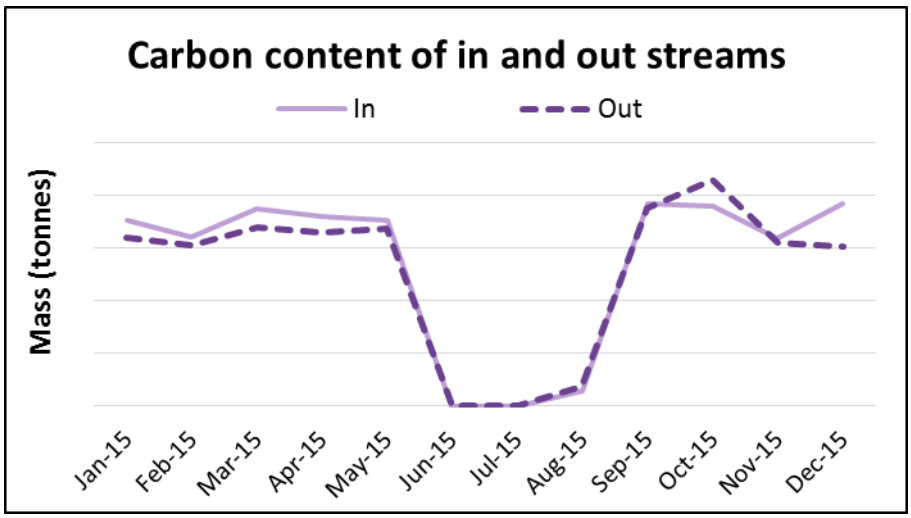


Figure E-2: Additional CS2 for Chapter 3 (Furnace 1)

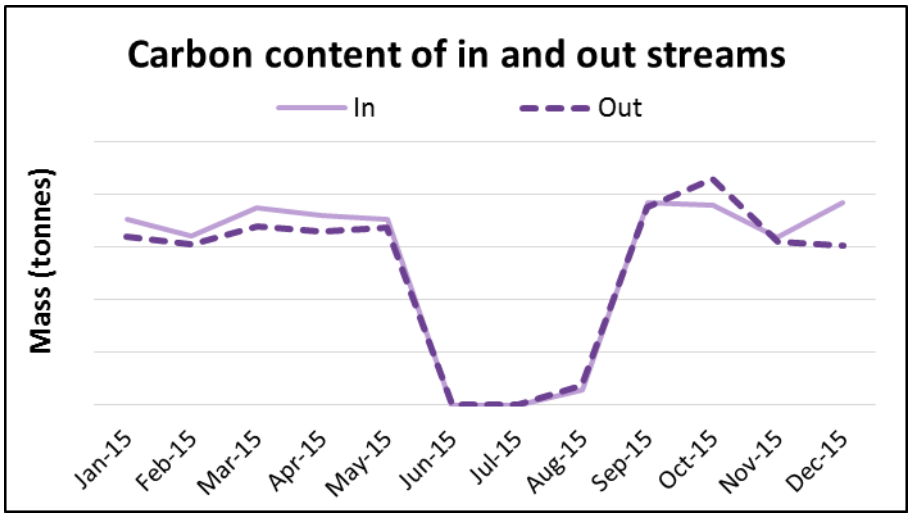


Figure E-3: Additional CS3 for Chapter 3 (Furnace 1)

Furnace 2:

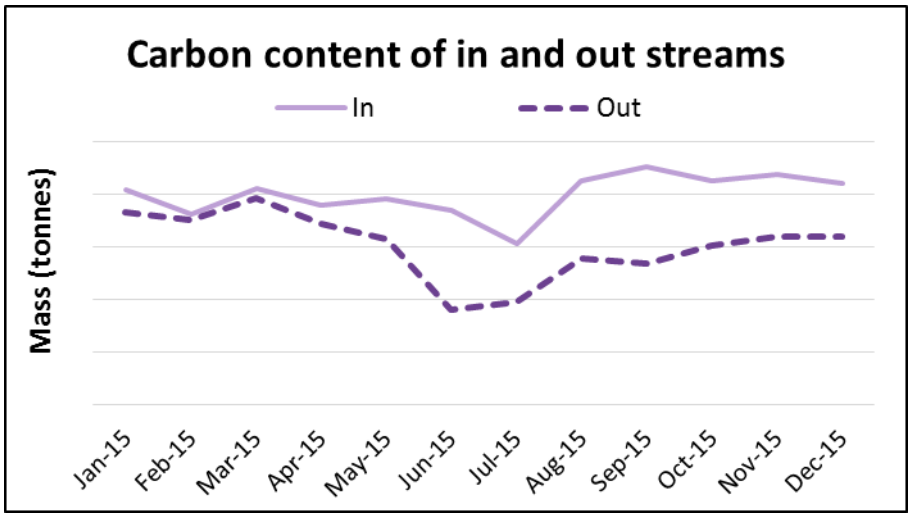


Figure E-4: Additional CS1 for Chapter 3 (Furnace 2)

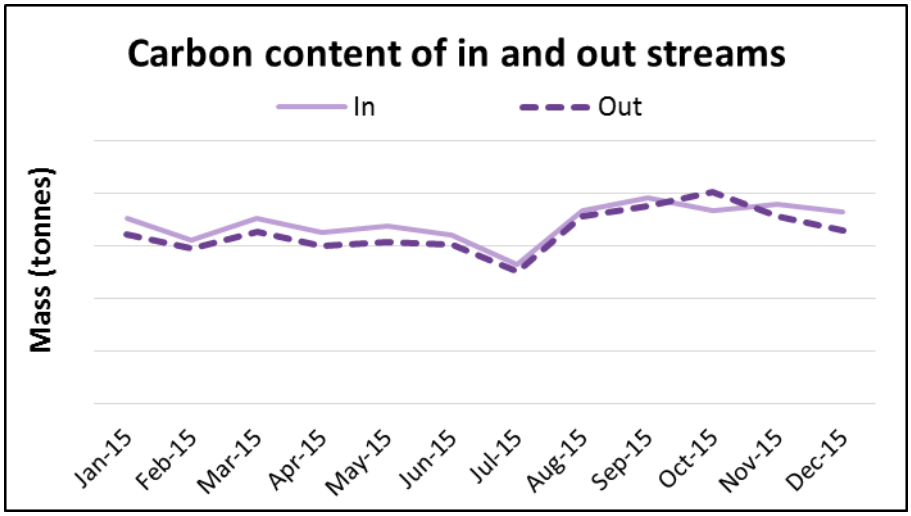


Figure E-5: Additional CS2 for Chapter 3 (Furnace 2)

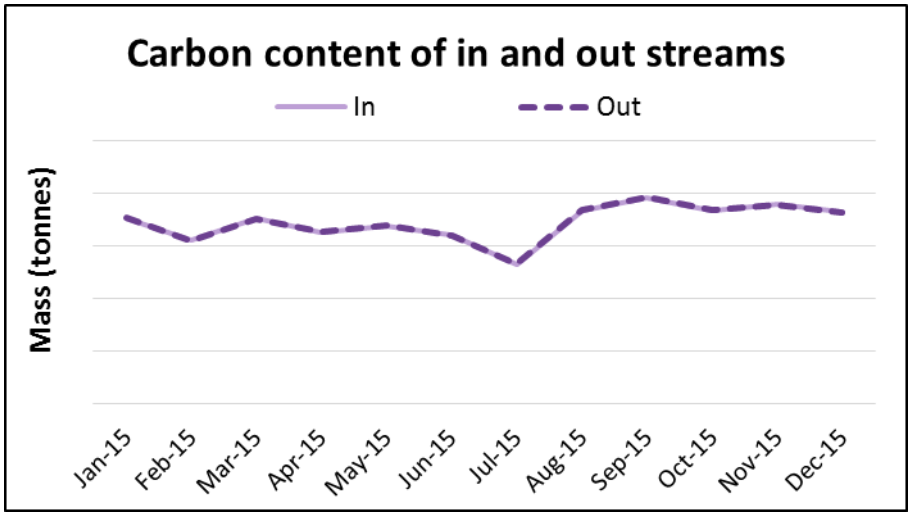


Figure E-6: Additional CS3 for Chapter 3 (Furnace 2)

Furnace 3:

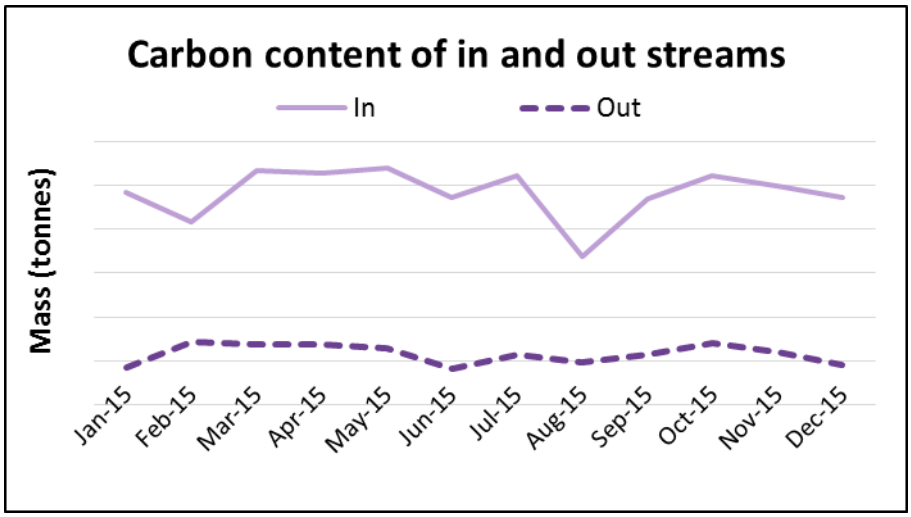


Figure E-7: Additional CS1 for Chapter 3 (Furnace 3)

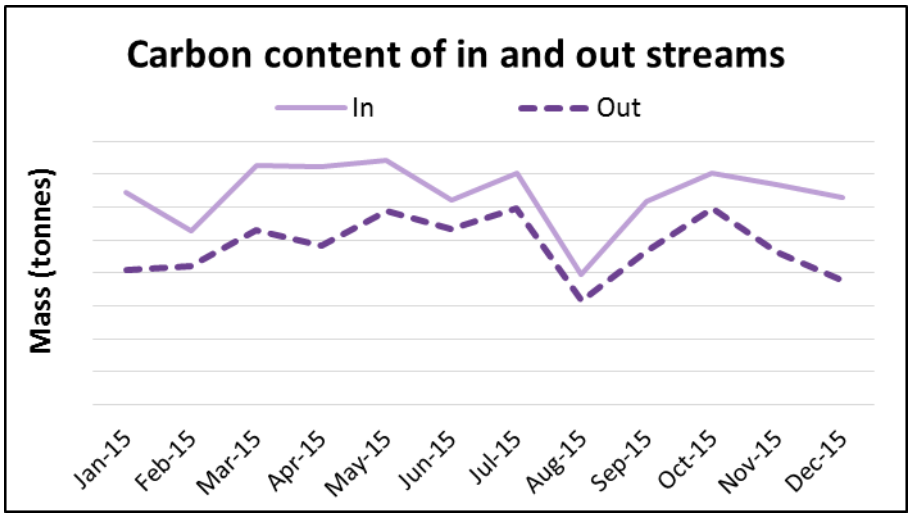


Figure E-8: Additional CS2 for Chapter 3 (Furnace 3)

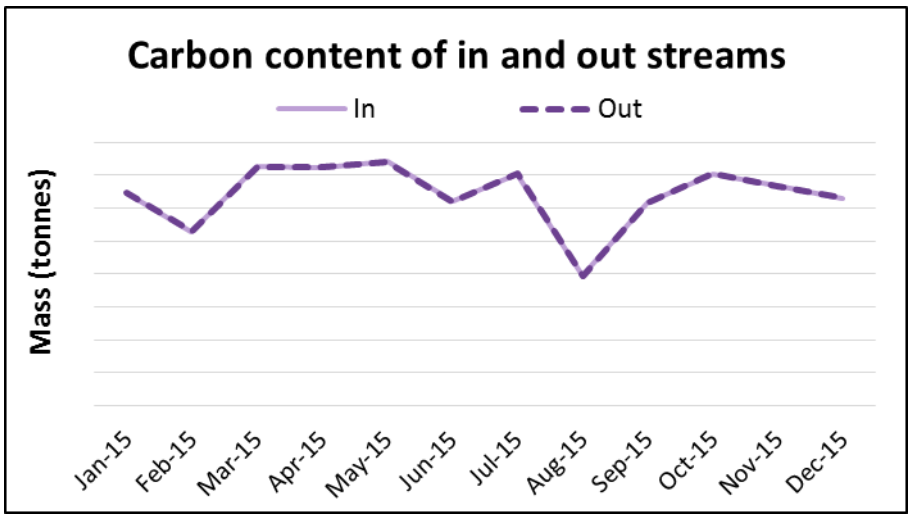


Figure E-9: Additional CS3 for Chapter 3 (Furnace 3)

Furnace 4:

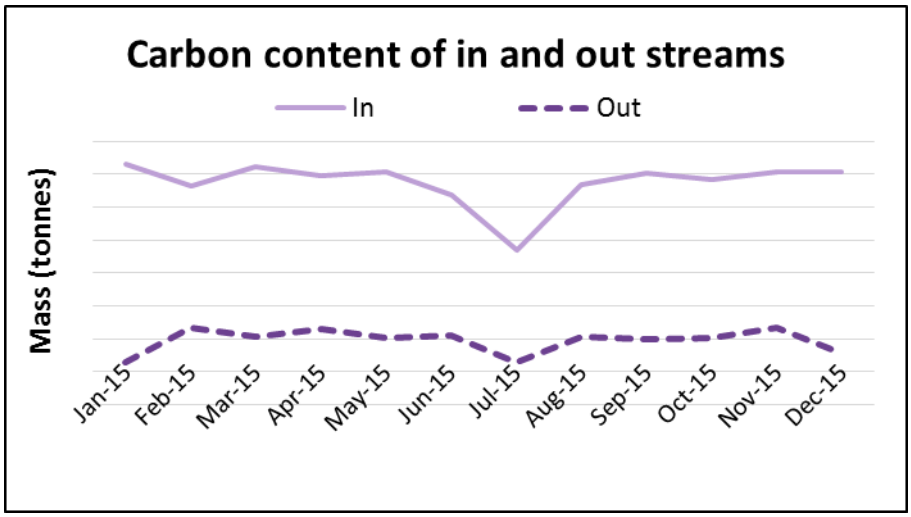


Figure E-10: Additional CS1 for Chapter 3 (Furnace 4)

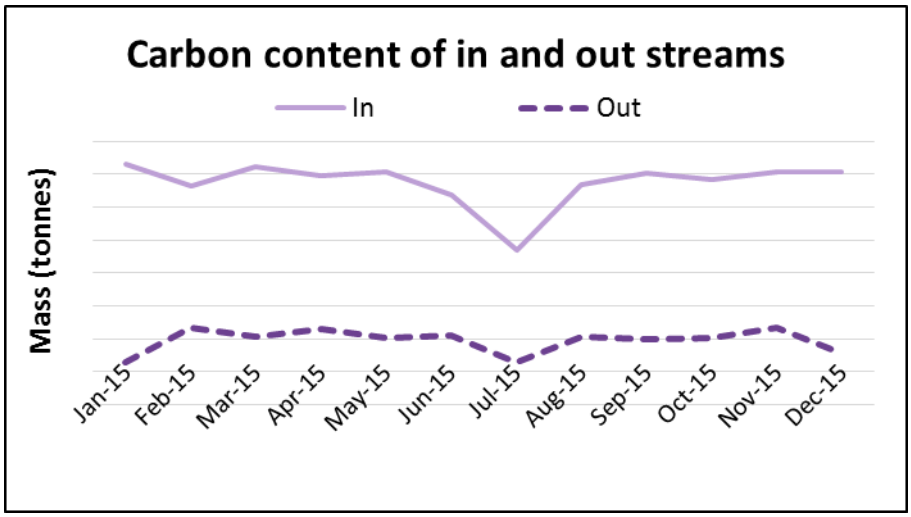


Figure E-11: Additional CS2 for Chapter 3 (Furnace 4)

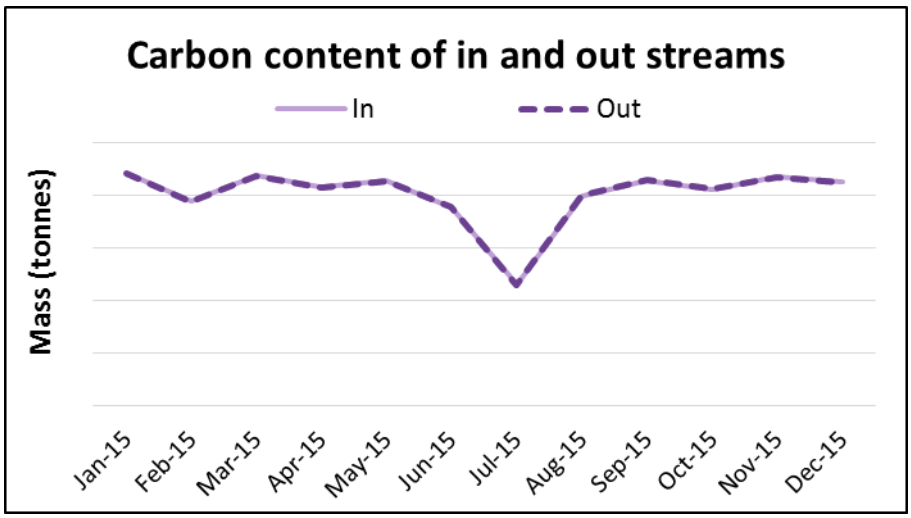


Figure E-12: Additional CS3 for Chapter 3 (Furnace 4)

Furnace 5:

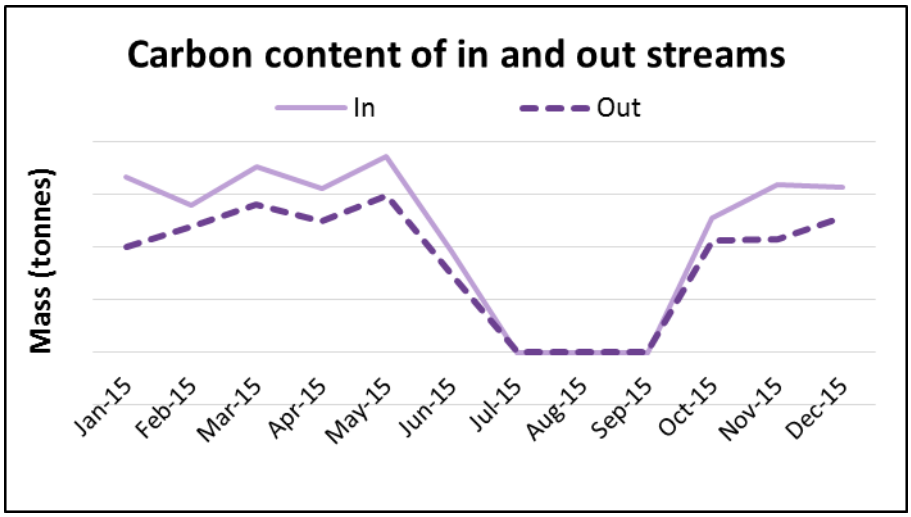


Figure E-13: Additional CS1 for Chapter 3 (Furnace 5)

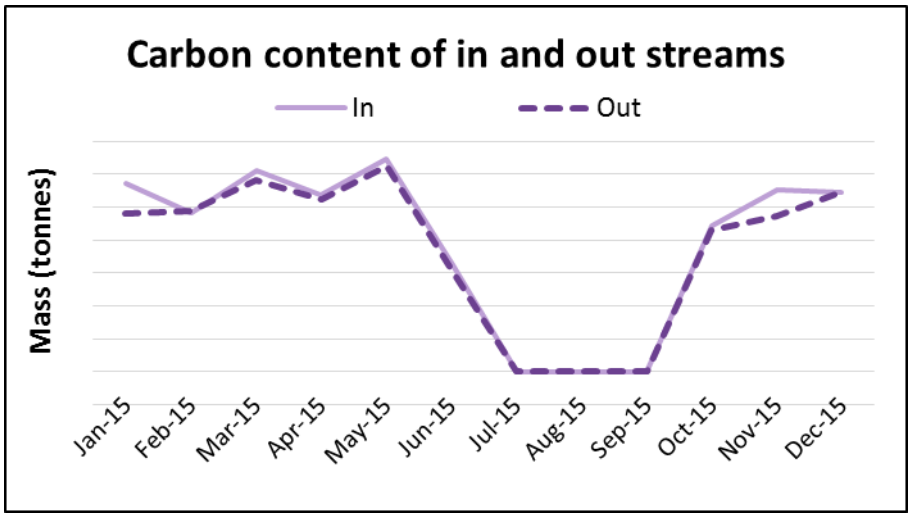


Figure E-14: Additional CS2 for Chapter 3 (Furnace 5)

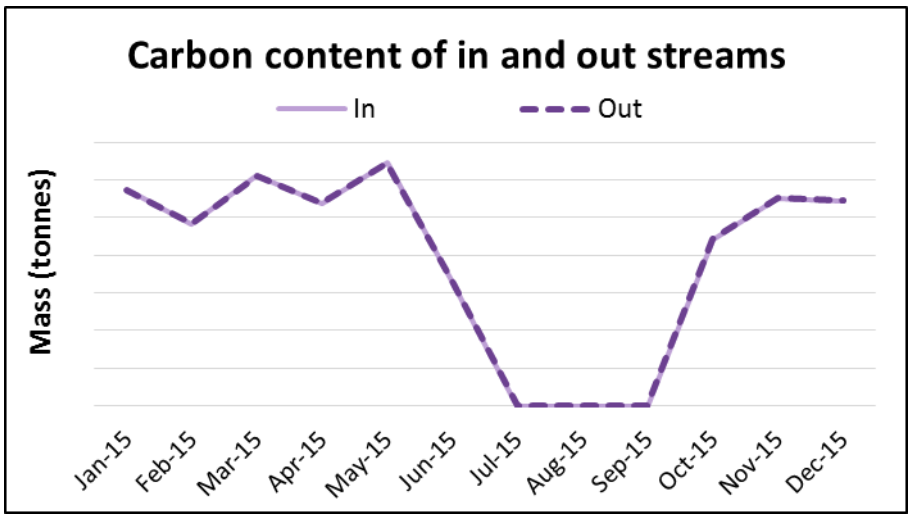


Figure E-15: Additional CS3 for Chapter 3 (Furnace 5)

Furnace 6:

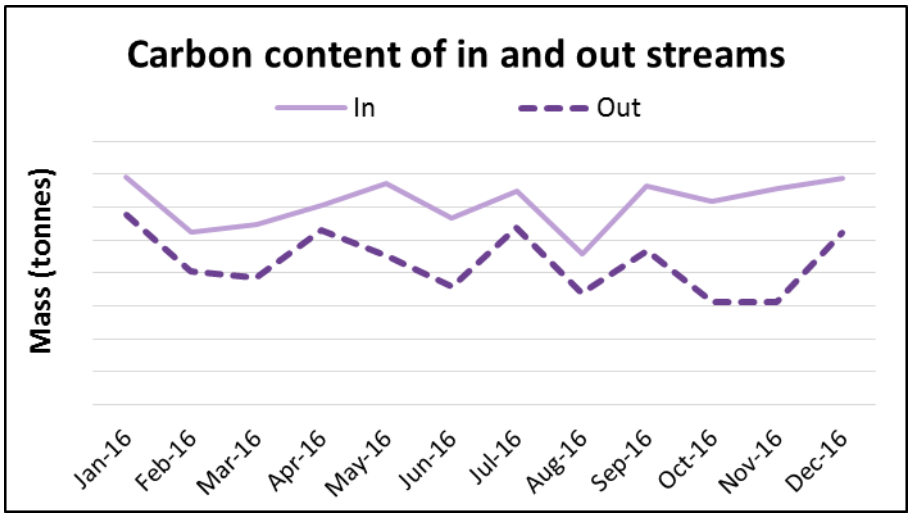


Figure E-16: Additional CS1 for Chapter 3 (Furnace 6)

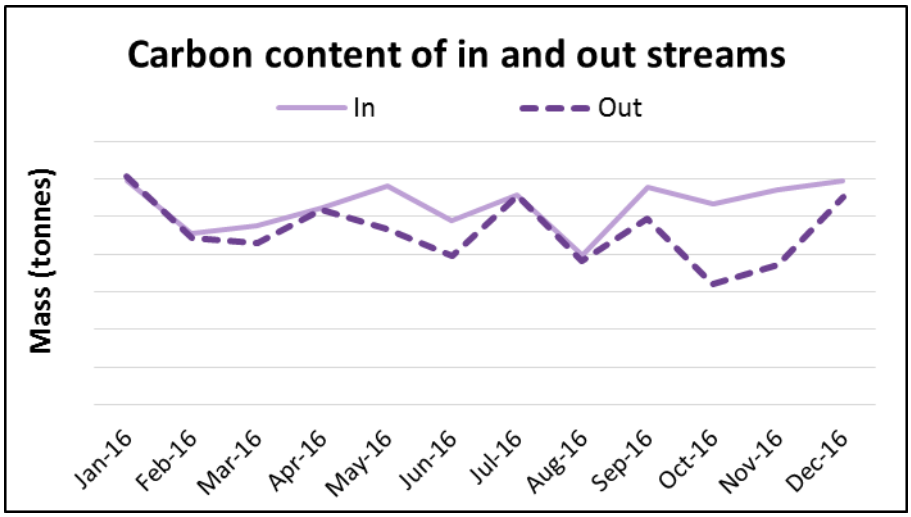


Figure E-17: Additional CS2 for Chapter 3 (Furnace 6)

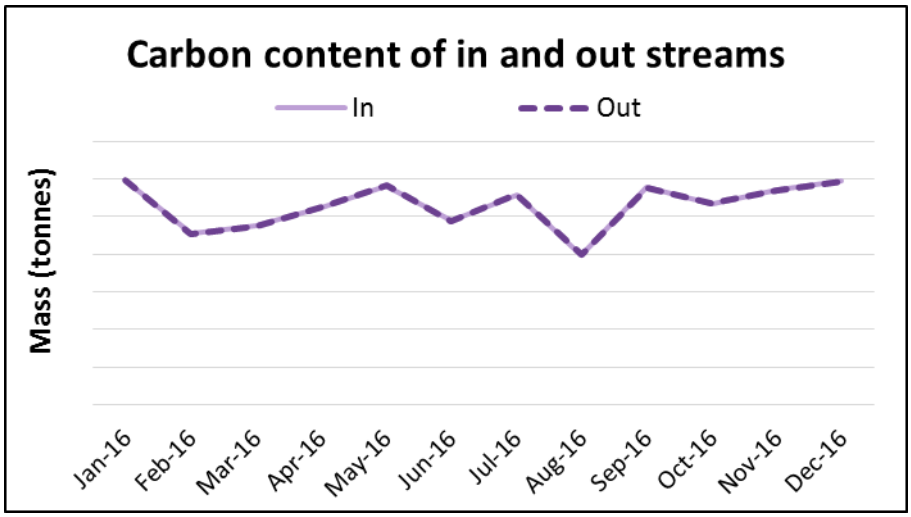


Figure E-18: Additional CS3 for Chapter 3 (Furnace 6)

Furnace 7:

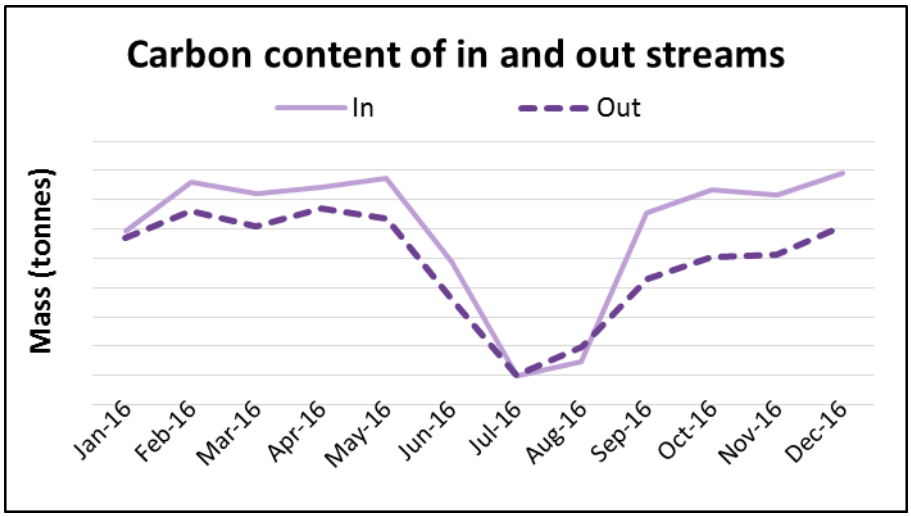


Figure E-19: Additional CS1 for Chapter 3 (Furnace 7)

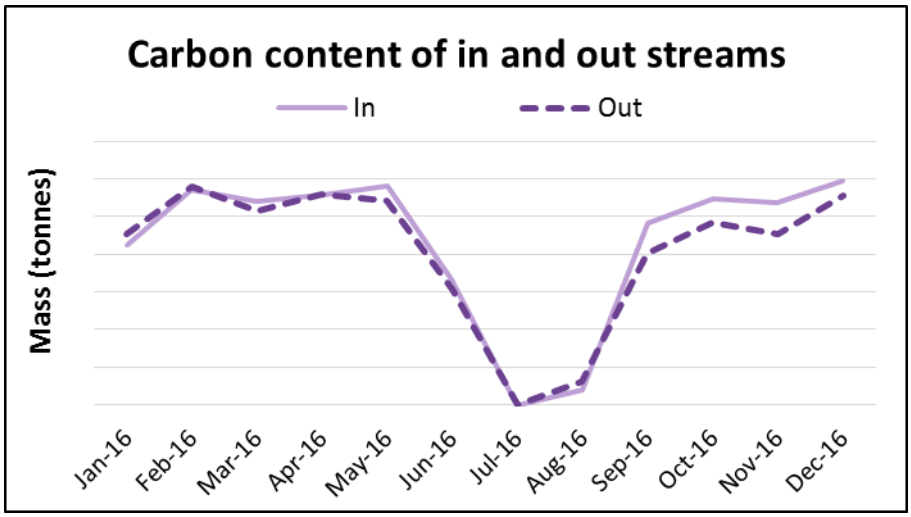


Figure E-20: Additional CS2 for Chapter 3 (Furnace 7)

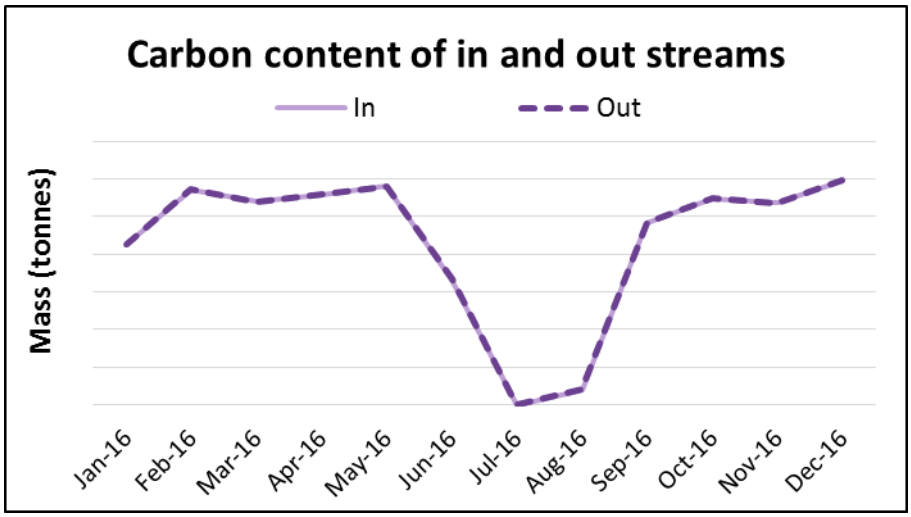


Figure E-21: Additional CS3 for Chapter 3 (Furnace 7)

Furnace 8:

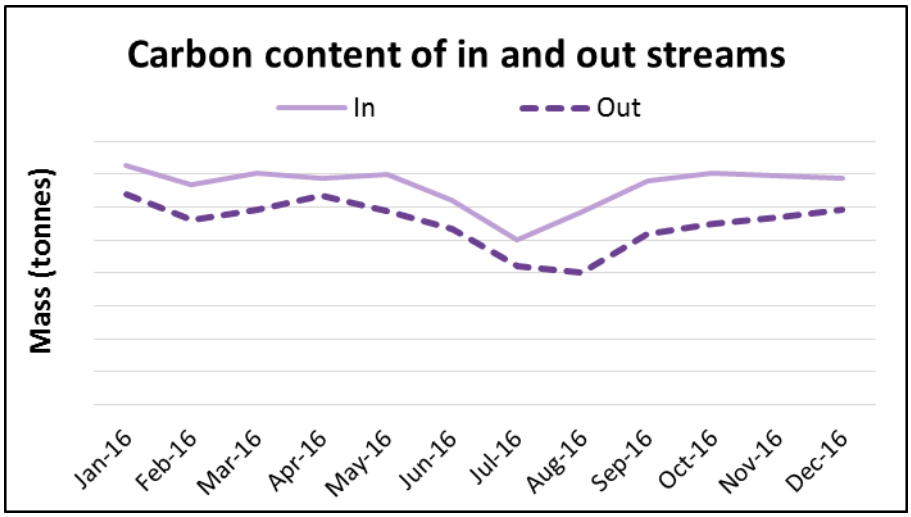


Figure E-22: Additional CS1 for Chapter 3 (Furnace 8)

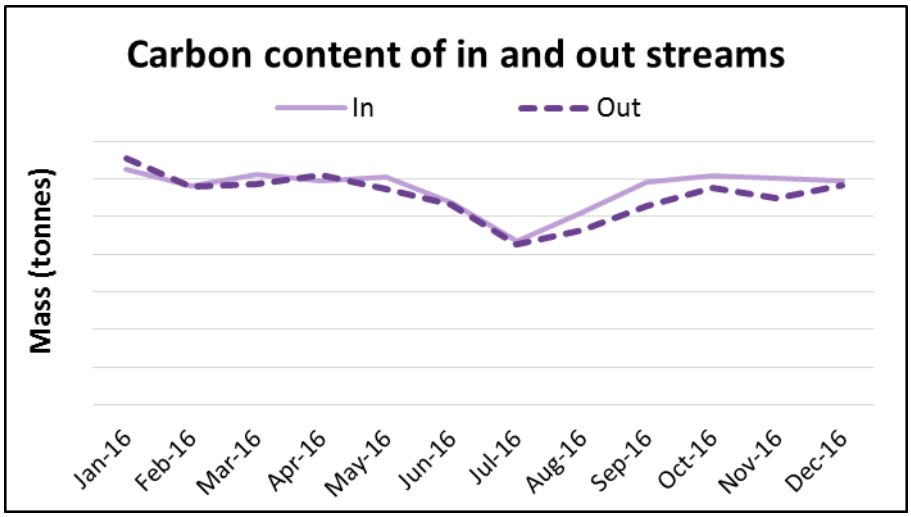


Figure E-23: Additional CS2 for Chapter 3 (Furnace 8)

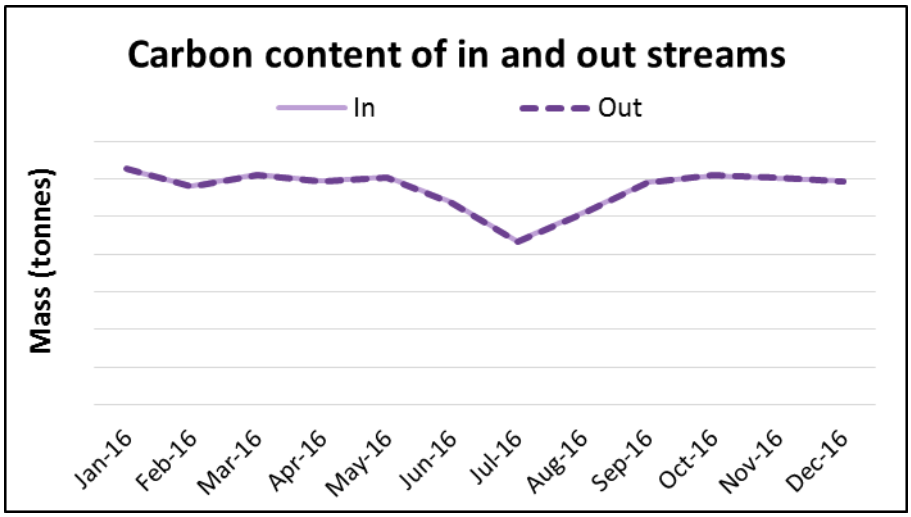


Figure E-24: Additional CS3 for Chapter 3 (Furnace 8)

Furnace 9:

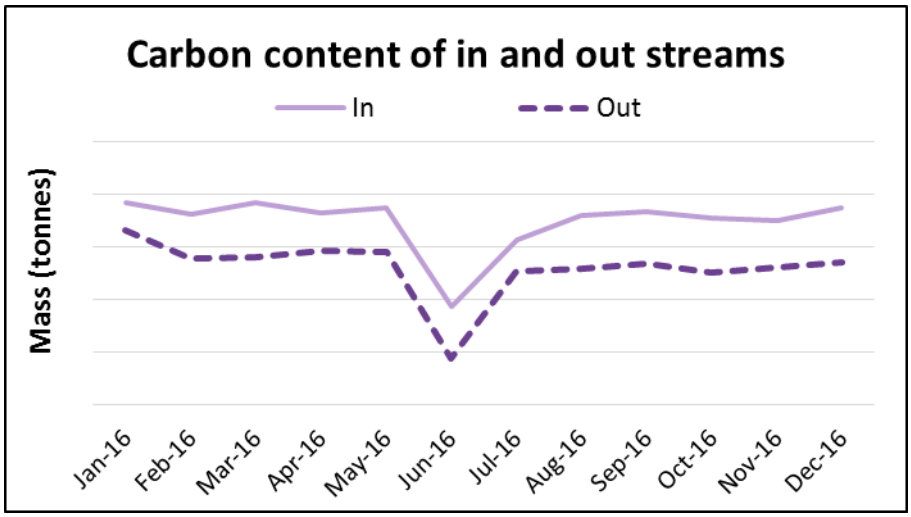


Figure E-25: Additional CS1 for Chapter 3 (Furnace 9)

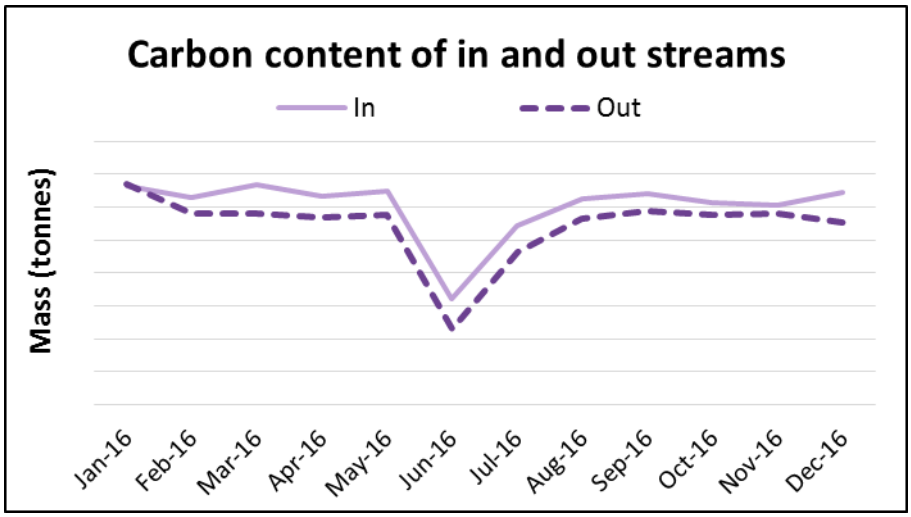


Figure E-26: Additional CS2 for Chapter 3 (Furnace 9)

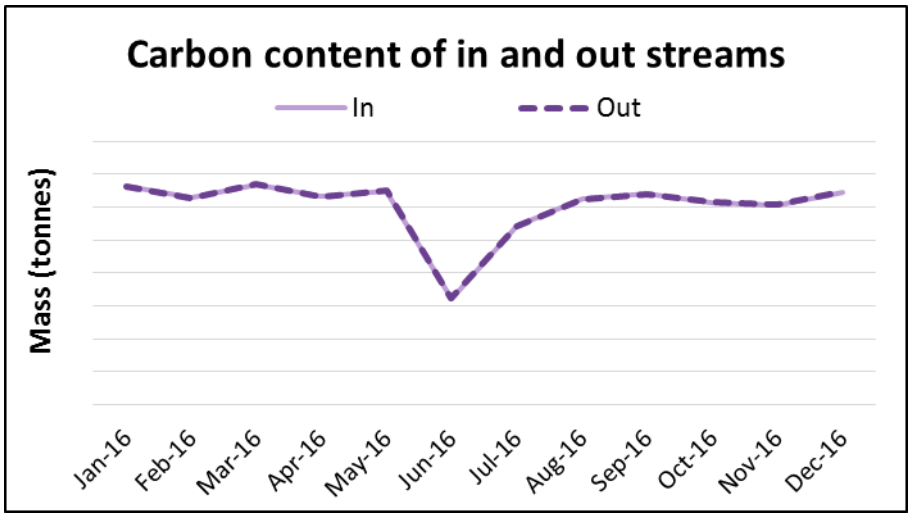


Figure E-27: Additional CS3 for Chapter 3 (Furnace 9)

Furnace 10:

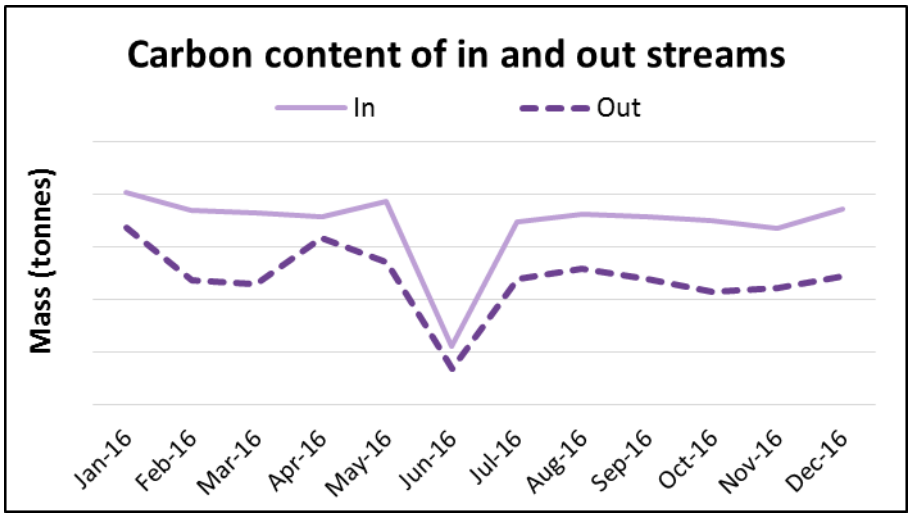


Figure E-28: Additional CS1 for Chapter 3 (Furnace 10)

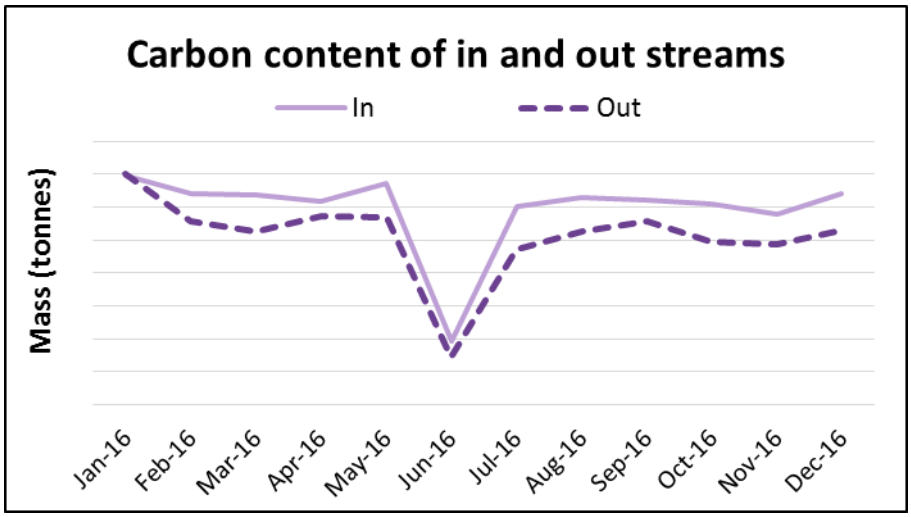


Figure E-29: Additional CS2 for Chapter 3 (Furnace 10)

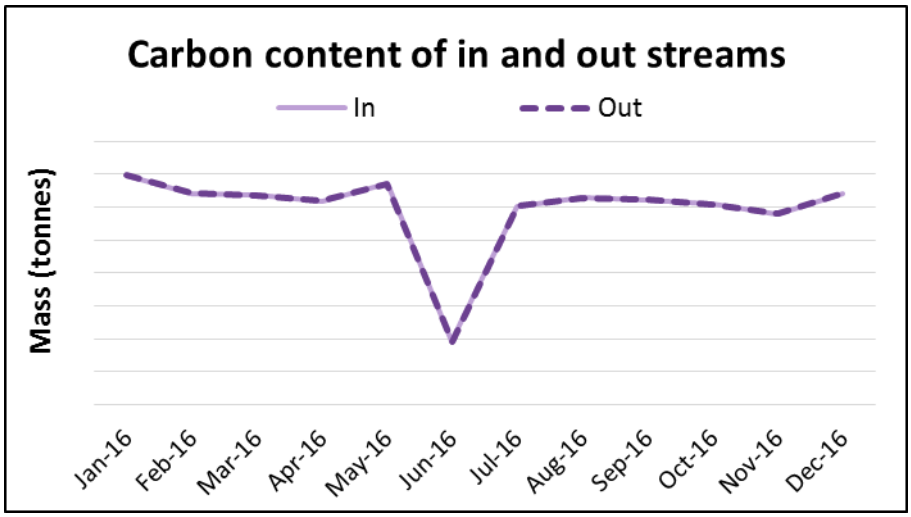


Figure E-30: Additional CS3 for Chapter 3 (Furnace 10)

Furnace 11:

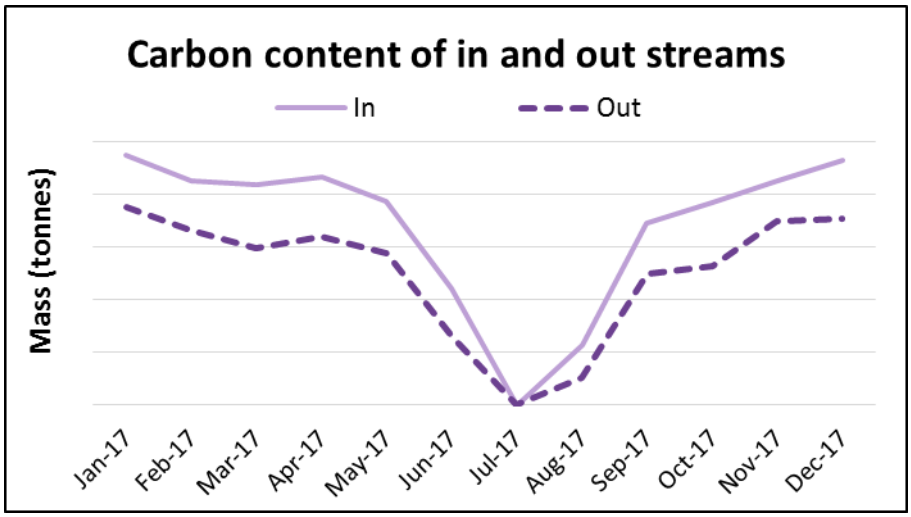


Figure E-31: Additional CS1 for Chapter 3 (Furnace 11)

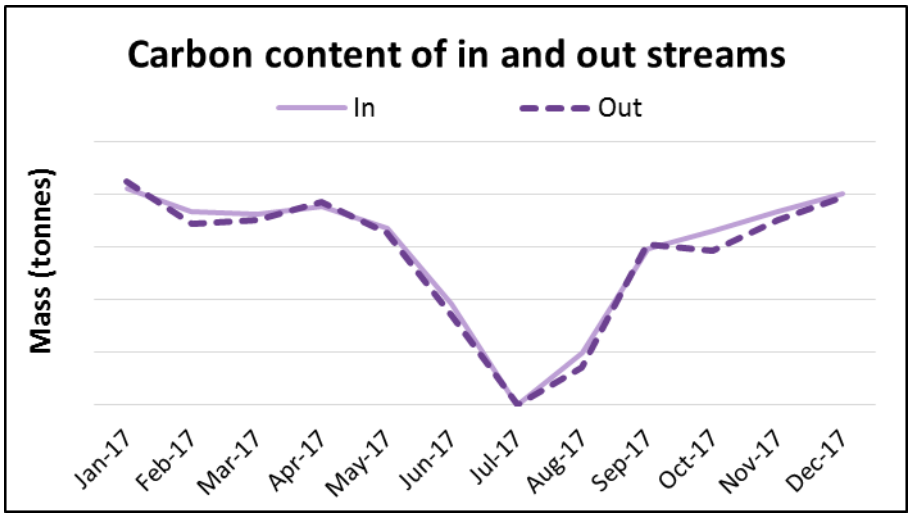


Figure E-32: Additional CS2 for Chapter 3 (Furnace 11)

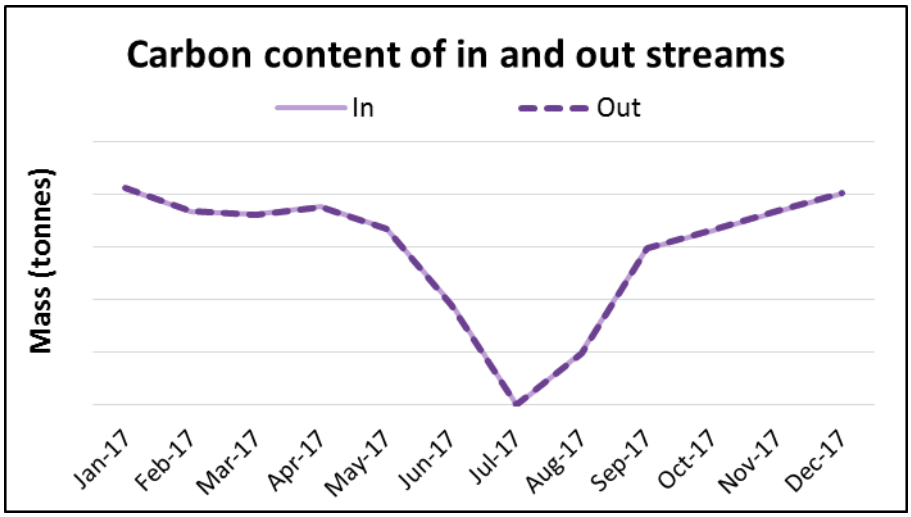


Figure E-33: Additional CS3 for Chapter 3 (Furnace 11)

Furnace 12:

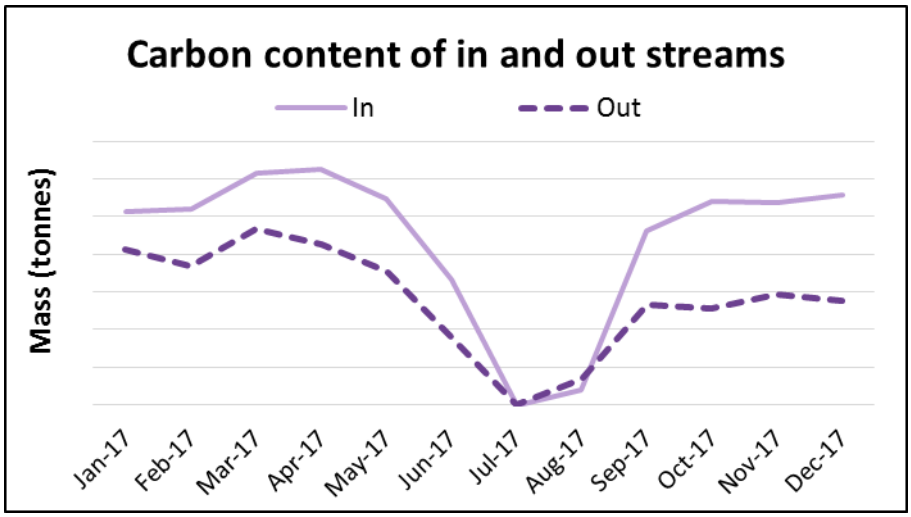


Figure E-34: Additional CS1 for Chapter 3 (Furnace 12)

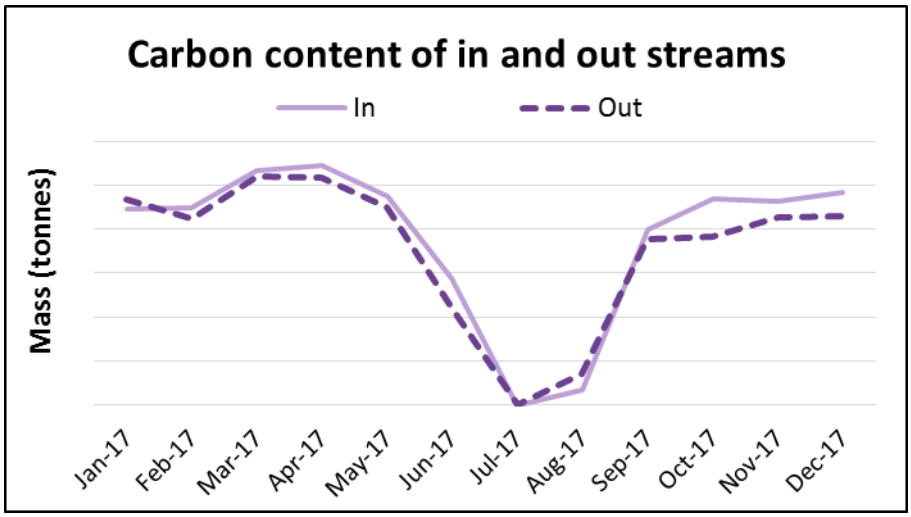


Figure E-35: Additional CS2 for Chapter 3 (Furnace 12)

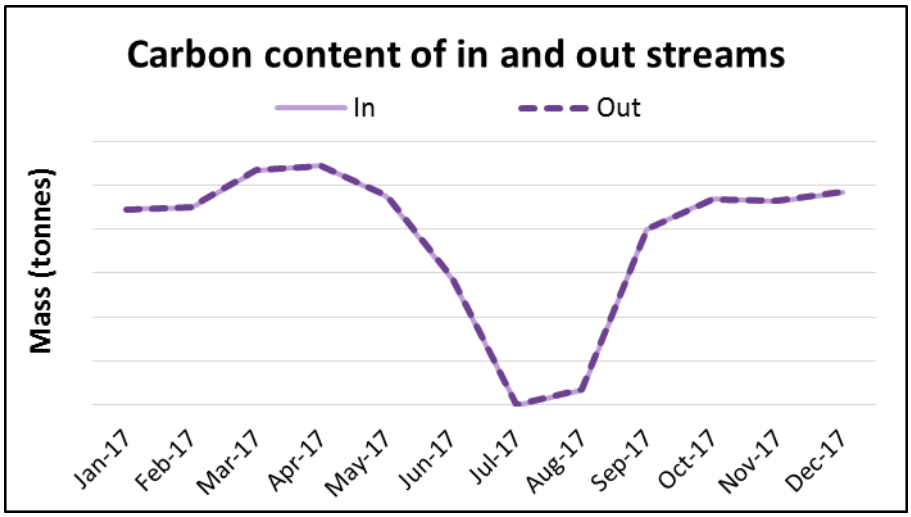


Figure E-36: Additional CS3 for Chapter 3 (Furnace 12)

Furnace 13:

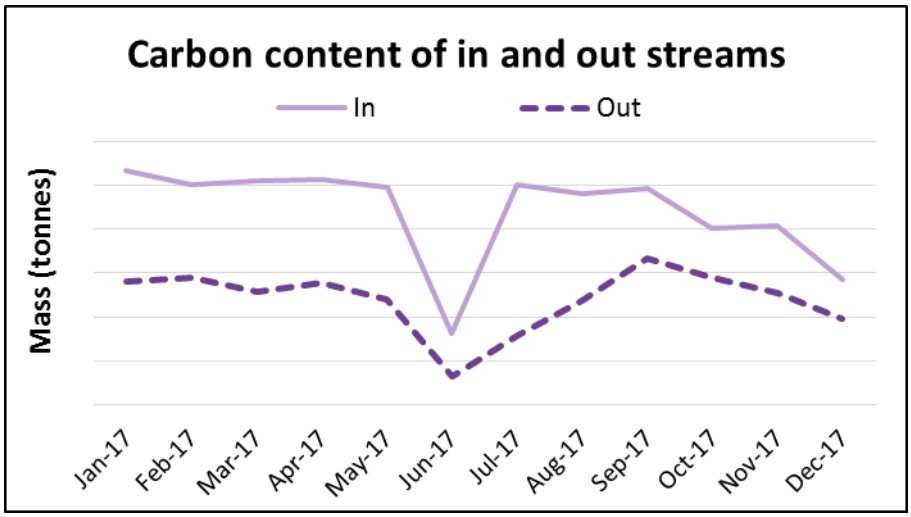


Figure E-37: Additional CS1 for Chapter 3 (Furnace 13)

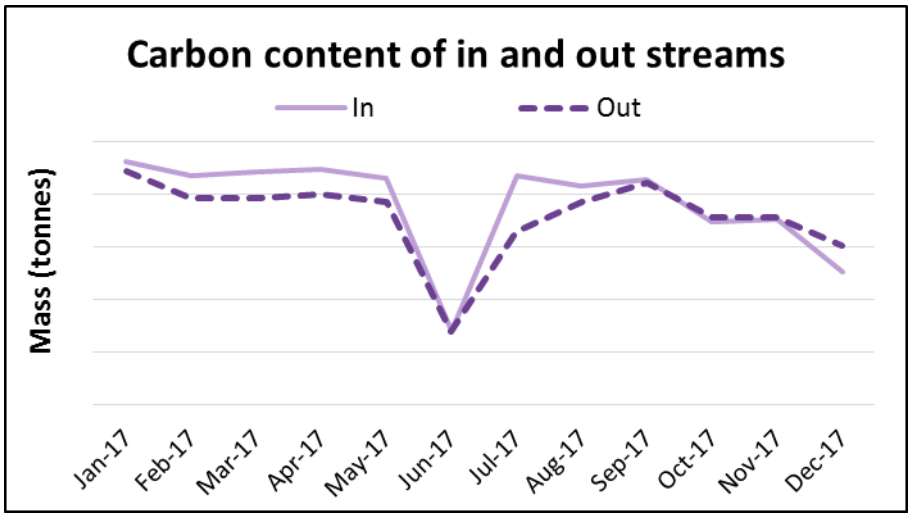


Figure E-38: Additional CS2 for Chapter 3 (Furnace 13)

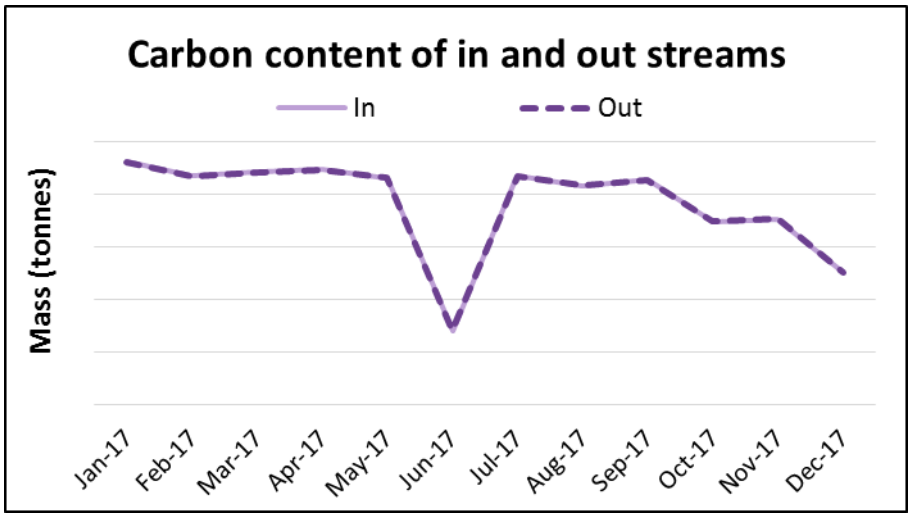


Figure E-39: Additional CS3 for Chapter 3 (Furnace 13)

Furnace 14:

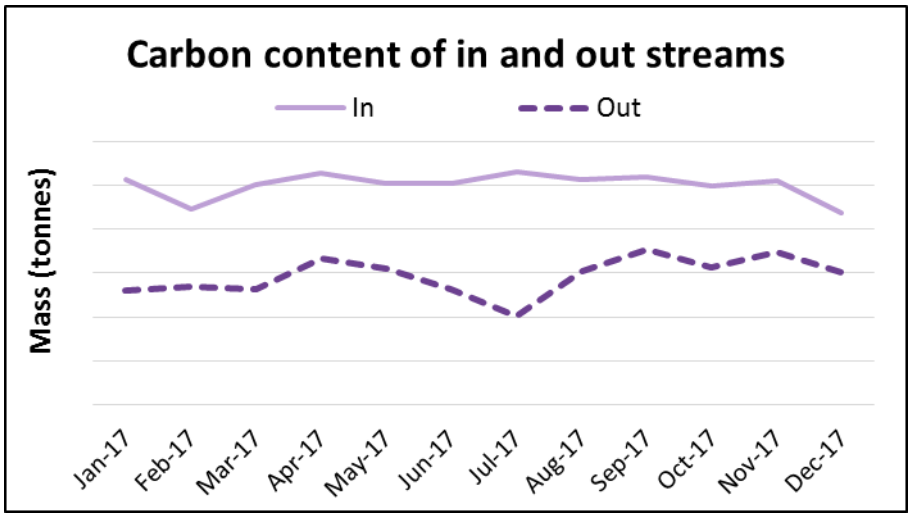


Figure E-40: Additional CS1 for Chapter 3 (Furnace 14)

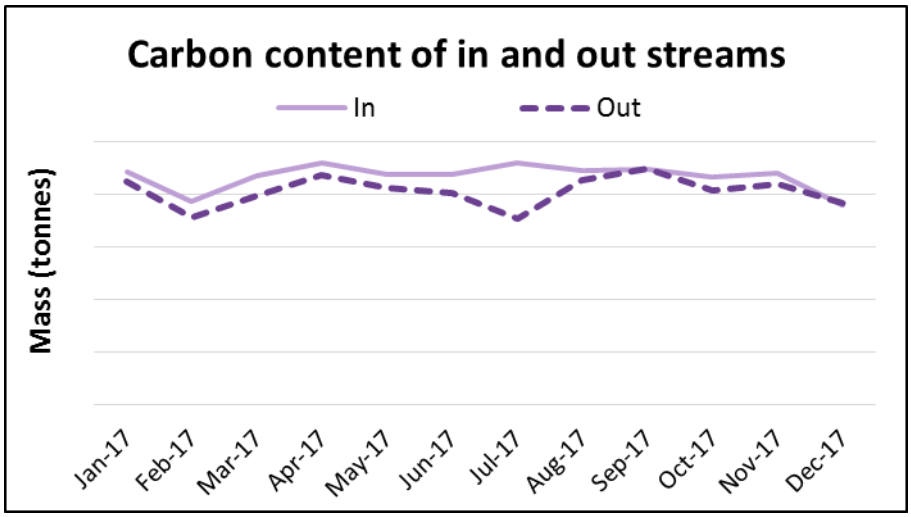


Figure E-41: Additional CS2 for Chapter 3 (Furnace 14)

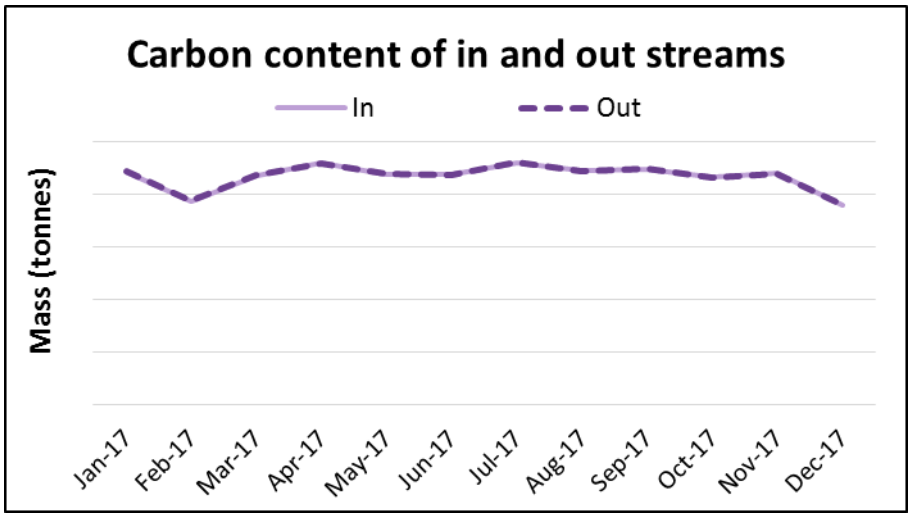


Figure E-42: Additional CS3 for Chapter 3 (Furnace 14)

Furnace 15:

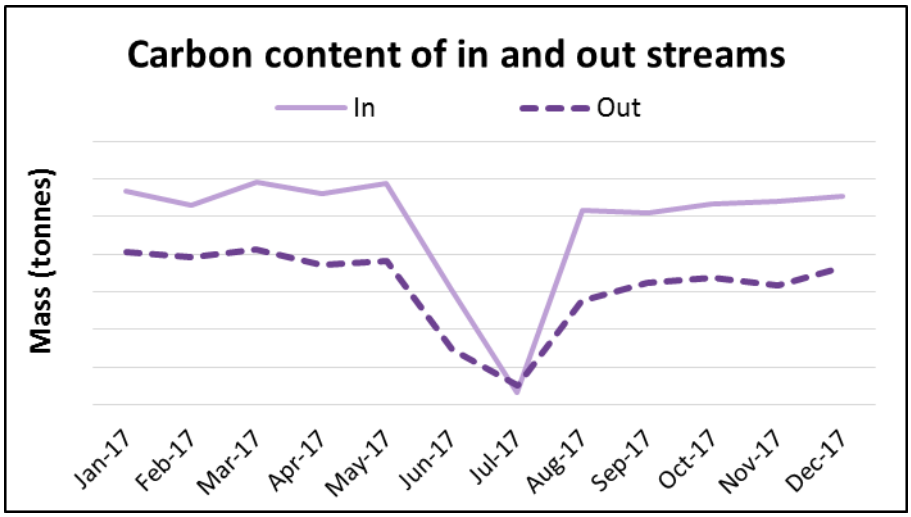


Figure E-43: Additional CS1 for Chapter 3 (Furnace 15)

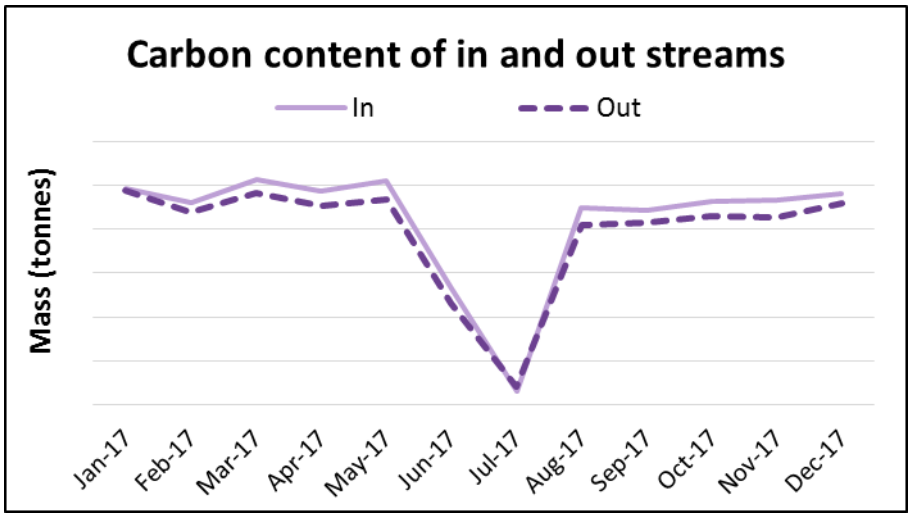


Figure E-44: Additional CS2 for Chapter 3 (Furnace 15)

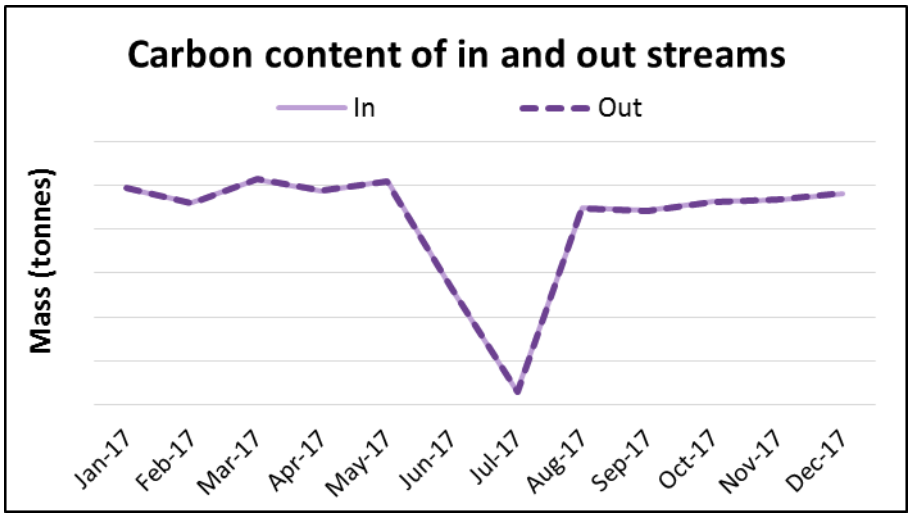


Figure E-45: Additional CS3 for Chapter 3 (Furnace 15)

Furnace 16:

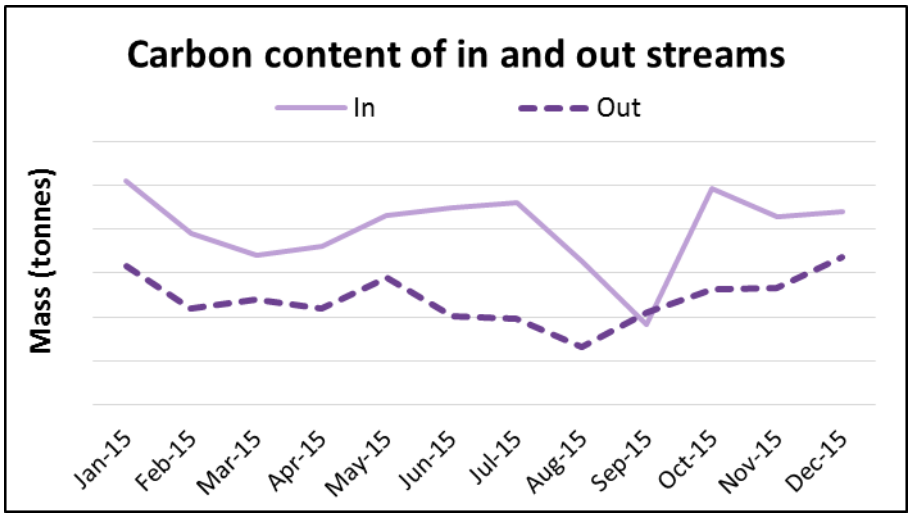


Figure E-46: Additional CS1 for Chapter 3 (Furnace 16)

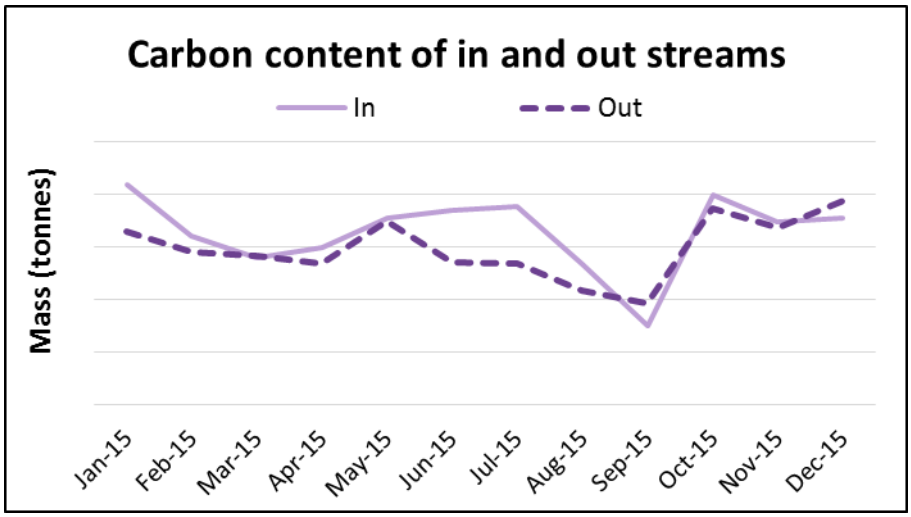


Figure E-47: Additional CS2 for Chapter 3 (Furnace 16)

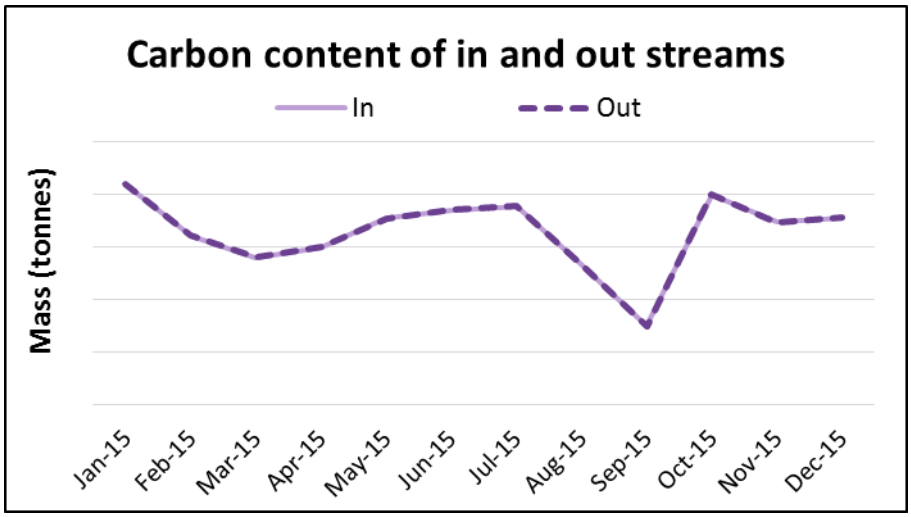


Figure E-48: Additional CS3 for Chapter 3 (Furnace 16)

F. APPENDIX F: Journal articles and conference papers

Two academic papers are attached (referred to in Section 5.2 – Novel contributions):

Appendix F.1:

- Journal article from the **South African Journal of Industrial Engineering (SAJIE):** K. Campbell, W. Booysen, J.C. Vosloo, "Evaluating the feasibility of the 12L tax incentive for energy-intensive industries", *SAJIE*, 2017.

Appendix F.2:

- Conference paper from the **Southern African Institute for Industrial Engineering (SAIIE):** K. Campbell, W. Booysen, M. Kleingeld, "Using data-driven analytics to develop a material balance over a ferrochrome furnace", *SAIIE*, 2018.

EVALUATING THE FEASIBILITY OF THE 12L TAX INCENTIVE FOR ENERGY-INTENSIVE INDUSTRIES

K. Campbell[1#*], W. Booysen[1†] & J.C. Vosloo[1]

ARTICLE INFO

Article details
Submitted by authors XX
Accepted for publication XX
Available online XX

Contact details
* Corresponding author
XX

Author affiliations
1 Centre for Research and Continued Engineering Development (CRCED), North-West University, Pretoria

\# Author was enrolled for a PhD degree in the Department of Mechanical and Nuclear Engineering at the North-West University's Centre for Research and Continued Engineering Development (CRCED) in Pretoria

† Author was a post-doctoral student at the North-West University's Centre for Research and Continued Engineering Development (CRCED) in Pretoria

DOI
http://dx.doi.org/10.7166/XXXX

ABSTRACT

Section 12L of the South African Income Tax Act (12L) aims to incentivise businesses to become more energy-efficient. However, claiming this benefit is a complex process that can become difficult, time-consuming, and costly if not clearly understood. It is therefore important to evaluate the feasibility of potential 12L applications before any unnecessary expenses are incurred or time is wasted. This article provides a brief overview of 12L and its associated literature before presenting a simplified feasibility evaluation strategy. The strategy consists of three key evaluation steps designed to identify potential issues quickly. The identified issues are linked to specific South African National Standards (SANS) guidelines to ensure that the issues can be resolved in a 12L-compliant manner. The strategy is applied to 47 industrial case studies. Some detailed results are presented to give a practical illustration of how the strategy works. The generalised results are further used to illustrate the potential benefit in time and cost reduction.

OPSOMMING

Artikel 12L van die Suid-Afrikaanse Inkomstebelastingwet (12L) beoog om besighede te stimuleer om meer energie-doeltreffend te word. Om hierdie voordeel te eis is egter 'n komplekse proses wat moeilik, tydrowend en duur kan word indien dit nie duidelik verstaan word nie. Dit is dus belangrik om die haalbaarheid van potensiële 12L-aansoeke te evalueer voordat enige onnodige uitgawes aangegaan word of tyd vermors word. Hierdie artikel bied 'n kort oorsig van 12L en die relevante literatuur, sodat 'n vereenvoudigde haalbaarheidsevalueringstrategie ontwikkel kan word. Die strategie bestaan uit drie sleutel evalueringstappe wat ontwerp is om vinnig moontlike kwessies te identifiseer. Die geïdentifiseerde kwessies word gekoppel aan spesifieke Suid-Afrikaanse Nasionale Standaarde (SANS) riglyne om te verseker dat die probleme op 'n 12L-voldoenbare wyse opgelos kan word. Die strategie word toegepas op 47 industriële gevallestudies. 'n Paar gedetailleerde resultate word aangebied om 'n praktiese illustrasie te gee van hoe die strategie werk. Die algemene resultate word verder gebruik om die potensiële voordeel in tyd- en kostevermindering te illustreer.

1 INTRODUCTION

South Africa is an energy-intensive country due to various mining and industrial activities [1]. In recent years, Eskom has struggled to keep up with constantly increasing energy demand. Mining and other large industries use about 45 per cent of the total national energy consumed within South Africa [2]. Ever since the country's energy supply became a concern, the government committed itself to promoting energy efficiency (EE), and so introduced the 12L tax incentive [3] [4].

The incentive aims to motivate companies to reduce their energy use and become more energy-efficient. The process of applying for such a tax deduction can, however, be very challenging [5] [6] (Steyn, M&V Standard for 12L tax incentives 2014). Strict rules must be adhered to when applying for the 12L deduction, as described in the National Tax Act [8], the Regulations [9], and the Standard [10]. Most importantly, the EE savings must be verified and the data must be traceable, accurate, and transparent.

This verification needs to be done by an independent SANAS (South African National Accreditation System) accredited measurement and verification (M&V) body, which can incur a significant financial expense [11]. There are only nine of these SANAS accredited M&V bodies in South Africa, making this a limiting factor [12]. Having only nine specialised bodies increases the potential costs of the application process.

Time is also a potential constraint when considering 12L. A company that demonstrates EE savings must complete its entire application within a certain timeframe — i.e., before the tax submission date. Another time restriction is that this incentive is only valid until 1 January 2020; in other words, there are only two full claimable years left. Therefore, no time should be wasted when applying for the deduction, meaning that the process needs to be completed as quickly and effectively as possible.

There is a need for a practical approach to evaluate the feasibility of potential 12L applications quickly, before an M&V body is officially involved. This will address the cost and time constraints by only submitting viable applications to the official process. However, it is also necessary to present solutions for applications that were deemed non-feasible. This work is based on a Masters dissertation submitted in 2017 [13].

2 LITERATURE REVIEW

2.1 Feasibility studies

Feasibility studies are usually performed when it is necessary to determine the viability of an idea for a new business opportunity [14] [15] [16] [17]. The main reason for such a study is to decide whether a certain project idea should be further investigated in more detail [18] [19]. When this is applied to the feasibility of the 12L tax incentive, the important question to ask is: will it be worthwhile to further investigate an opportunity for 12L? A generic list of steps on how to do a feasibility study is constructed after the necessary research has been done [14] [16] [17] [20] [21] [22]. These steps are listed below:

- Define the opportunity
- Determine the requirements
- Identify any competition
- Conduct an assessment
- Ask: Is there a financial benefit?
- Ask: Is there sufficient technology?
- Identify possible risks
- Address risks identified with possible solutions

These steps will be used to develop an in-detail strategy for evaluating the feasibility of the 12L tax incentive for energy-intensive industries.

2.2 Section 12L tax incentive

The South African National Energy Development Institute (SANEDI) has been selected as the Section 12L official. They have the responsibility of appointing suitably qualified persons to ensure that an EE savings report [9]:

- complies with the Section 12L Regulation,
- complies with the SANS 50010 M&V Standard, and
- is an accurate and conservative reflection of the actual EE savings.

If, and when, SANEDI is fully satisfied that all requirements are met, they must issue a certificate to the entity claiming the allowance.

2.2.1 Quantification of 12L potential

Energy savings must be calculated by comparing the measured use of energy before and after the implementation of a certain energy savings measure. The savings must also be determined by making suitable adjustments to account for possible changes in the relevant conditions [10].

According to the SANS 50010 [10], energy savings can be calculated by comparing the measured energy use before and after an energy savings intervention. This is done with the following equation:

$$E_s = E_{BL} - E_{PA} \pm E_{adjustments} \quad \text{(Equation 1)}$$

The figure below provides a visual representation to explain what is meant by the terms savings (E_S), baseline (E_{BL}), assessment (E_{AP}), and adjustments (E_{adj}) [10].

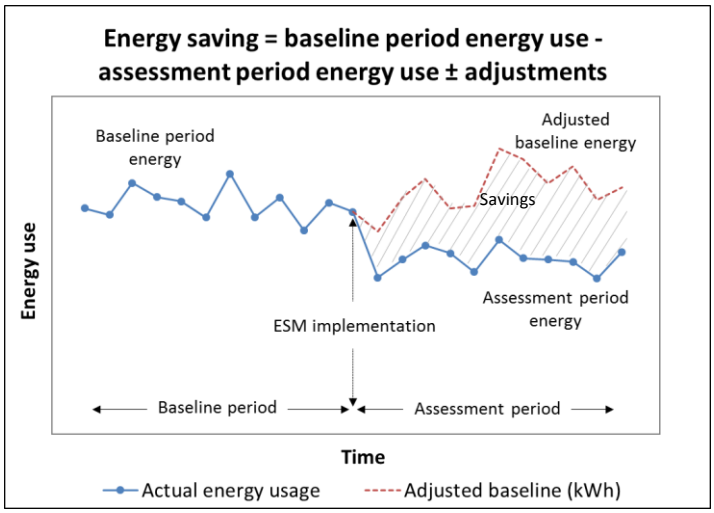


Figure 1: Graphical overview of EE determination

The energy savings of a certain entity can be determined by comparing the energy used before and after implementation. This can be done using different methods when making adjustments for process changes. This section will focus on two specific EE savings calculation methods: a) energy intensity calculations, and b) regression models [23].

a) Intensity calculations

An energy intensity calculation is a simple way of calculating the energy savings, and is suitable for data with a low resolution (fewer data points). This is simply done by using the next three equations: annual energy intensity (Equation 2), adjusted BL energy consumption (Equation 3), and annual energy savings (Equation 4):

$$I_{BL} = \frac{E_{BL}}{P_{BL}} \quad \text{(Equation 2)}$$

$$E_{BL\,(adjusted)} = P_{AP} \times I_{BL} \quad \text{(Equation 3)}$$

$$E_{savings} = E_{BL\,(adjusted)} - E_{AP} \quad \text{(Equation 4)}$$

where E_{BL} = baseline energy consumption, P_{BL} = baseline production, P_{AP} = assessment production, E_{AP} = actual assessment energy consumption. If $E_{savings}$ are negative, it means that there have been no significant EE improvements. However, a positive $E_{savings}$ value indicates 12L potential.

b) Regression model calculations

This calculation is recommended for a more accurate result, especially if higher data resolution is available. In order to calculate EE savings through the regression model, the following steps are required:

- Define the baseline model
- Determine the predicted energy usage
- Calculate the energy savings for each data point
- Calculate the total annual energy savings

Defining the baseline model includes plotting the baseline values on a graph (energy driver, e.g. production = x-values; energy carriers, e.g. electricity consumption = y-values). A linear regression line is then drawn through the data points, according to Equation 5:

$$y = mx + c \qquad \text{(Equation 5)}$$

where *y* represents the predicted energy consumption at a certain data point, while *x* symbolises the energy driver. The slope of the regression line is indicated by *m*, while *c* is the intercept of the line.

Calculating the energy savings for each data point is done by simply subtracting the actual energy consumption from the predicted energy consumption (as described by Equation 4) for every data point.

2.2.2 Summary of 12L requirements

From the necessary research conducted, it can be concluded that, when applying for the 12L tax allowance, many rules and requirements need to be adhered to. Essentially, data is one of the most important aspects of the 12L requirements:

- Data requirements: the BL and AP energy **data needs to be accurate**.
- Calculating EE savings: **accurate data** is necessary to construct the correct baseline model, which is then used to calculate the energy savings.
- Limitations and concurrent benefits: sufficient **data management** is needed in order to identify, and quantify, any limitations or concurrent benefits that may apply.

Thus, the quality of data is an important factor when claiming the 12L tax allowance. The next section will focus on the management of data and data quality in general.

2.3 Quality management systems (QMSs)

Having an accurate and transparent 12L application primarily depends on the data quality for the specific site. The manner in which the data is measured, processed, verified, and managed is significant for data quality. Below is a flow diagram (Figure 2) that has been created in order to illustrate the aspects of data quality.

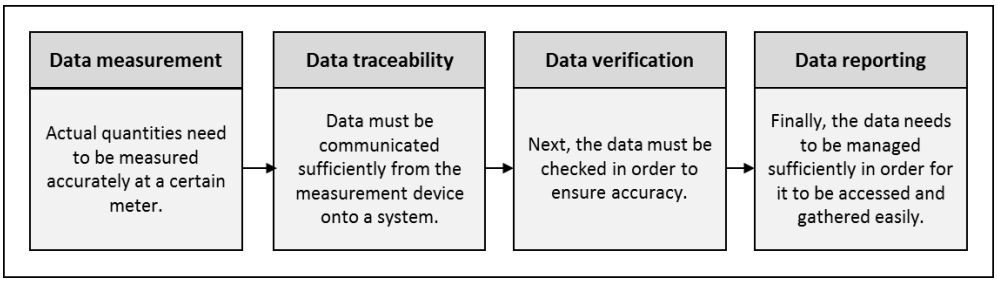


Figure 2: Aspects of data quality

Based on the flow diagram, it is clear that there are several areas where data related issues may arise during a 12L investigation. These four aspects have been investigated, and will be addressed on the basis of various national and international standards.

The following table summarises some standards that can be used to address various 12L data-related issues [10] [24] [25] [26] [27].

Table 1: Summary of standards addressing data issues for 12L requirements

Issue	How the 12L regulation highlights this issue	Standard in which this issue is addressed
Data measurement	*"If SANEDI is satisfied that the information contained in a report is an **accurate** reflection of the EE savings…" (p.7)*	ISO 9001:2008
		ISO 14001:2004
		ISO 50001:2011
		SANS 50010:2011
Data traceability		ISO 8000:2011
		ISO 9001:2008
		ISO 14001:2004
		ISO 50001:2011
Data verification		ISO 9001:2008
		ISO 50001:2011
Data reporting	*"The certificate issued by SANEDI … must contain": BL energy, PA energy, EE savings/delta energy, M&V details, applicant and tax details (p.8)*	SANS 50010:2011 SANS 50001

It is clear from this table that various standards are available to address the four main data issues for the 12L requirements.

2.4 Summary of literature review

Information about the feasibility studies was collected and summarised. The summary provided a general method for how feasibility studies are usually approached, based on the previous studies. After a literature study had been performed (regarding *Regulations of 12L* and *Quality management systems*), it was found that this general method could be applied specifically to 12L. This method for a generic feasibility study is applied to a 12L investigation, and is outlined below:

- ***Define opportunity:*** Opportunity to claim 12L
- ***Determine requirements:*** EE savings, as well as accurate and reliable data, are compulsory
- ***Identify competition:*** Competition includes limitations and concurrent benefits (e.g., 12I, PPA)
- ***Conduct an assessment:*** Calculate preliminary EE savings
- ***Is there a financial benefit?*** Financial benefit due to savings?
- ***Is there sufficient technology?*** Sufficient data basis technology or data management system to deliver reliable data? Data management?
- ***Identify possible risks:*** Having no savings or unreliable or inaccurate data are both potential risks
- ***Address risks identified with possible solution:*** Implementation of a quality management system

This method will be used to develop a strategy for evaluating the feasibility of the 12L tax incentive for energy-intensive industries. The final strategy will be used throughout the rest of this study.

3 METHODOLOGY

The methodology is divided into three divisions or main phases: quantifying EE savings; evaluating data compliance; and addressing potential compliance issues. An overview of this strategy is presented in Figure 3 (below).

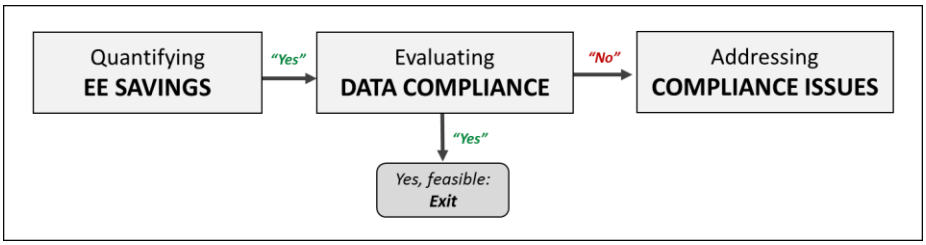


Figure 3: Basic three-step strategy for evaluating 12L feasibility

This strategy will provide the 12L applicant with a holistic approach to conducting an initial internal investigation before any unnecessary expense or time is wasted. This strategy can therefore serve as a practical application to investigate the possibility of claiming the 12L tax incentive. Each step will now be discussed in more detail.

3.1.1 PHASE 1: Quantifying EE savings

Phase 1 of the strategy presents the steps required to quantify the preliminary EE savings; this is presented in Figure 4.

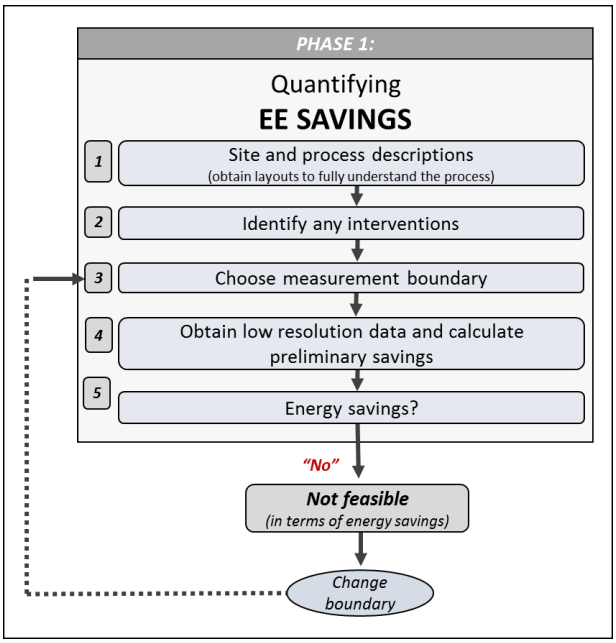


Figure 4: PHASE 1 — Quantifying EE savings

If there is a potential for a 12L claim (recommended as 1 GWh [28]), the applicant may proceed to the next phase (*evaluating data compliance*). If sufficient savings do not show, other boundary options can be evaluated. The investigation may be terminated if no potential is found.

3.1.2 PHASE 2: Evaluating data compliance

Having an accurate and transparent 12L application is essential. It is important that all the data used to calculate the EE savings for the 12L application accurately reflects the truth. The manner in which the data is measured, processed, used, and verified are all key factors to consider when evaluating data compliance. Phase 2 of the strategy is presented in Figure 5.

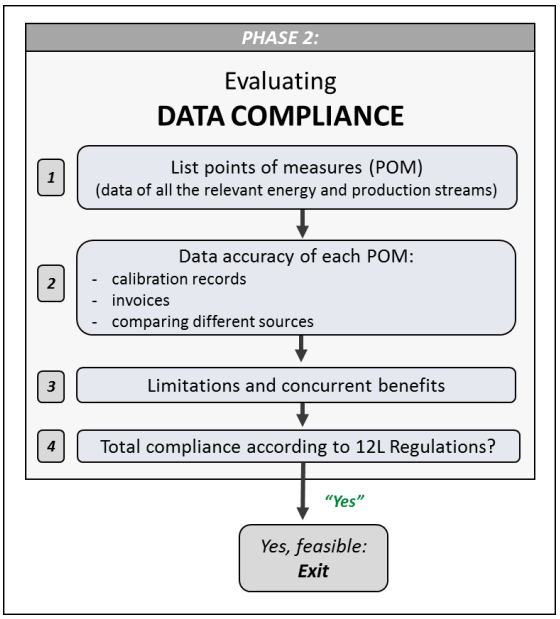


Figure 5: PHASE 2 — Evaluating data compliance

If thorough compliance cannot be proven, the applicant must proceed to *Phase 3* (addressing compliance issues). It is assumed that non-compliance is generally due to inaccurate, unverified data, or the presence of a limitation or concurrent benefit.

3.1.3 PHASE 3: Addressing compliance issues

This section will provide ways to address the lack of data compliance. The suggested improvements are done on the basis of quality management systems (QMSs), as discussed in Section 2.3. The basic process of addressing potential problems is provided in Figure 6.

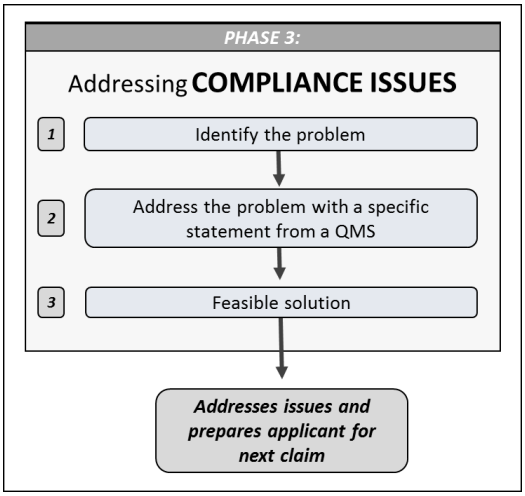


Figure 6: PHASE 3 — Addressing compliance issues

The last step of Phase 3 can be done using a condensed version of Table 1 (presented in Table 2). This table provides a quick and effective way to identify certain international standards that would address one of the issues regarding data compliance.

Table 2: Addressing compliance issues with specific QMSs

	ISO 8000	ISO 9001	ISO 14001	ISO 50001	ISO 50010
Data measurement		x	x	x	x
Data traceability	x	x	x	x	
Data verification		x		x	
Data reporting				x	x

The final step of the strategy ensures that the identified issues are addressed, and that a *feasible solution* will eventually be achieved. This will prevent the issues from developing again in the future and will, therefore, prepare the applicant for the next claim.

3.1.4 FINAL STRATEGY

The three phases can be combined to present the final strategy (presented in Figure 7).

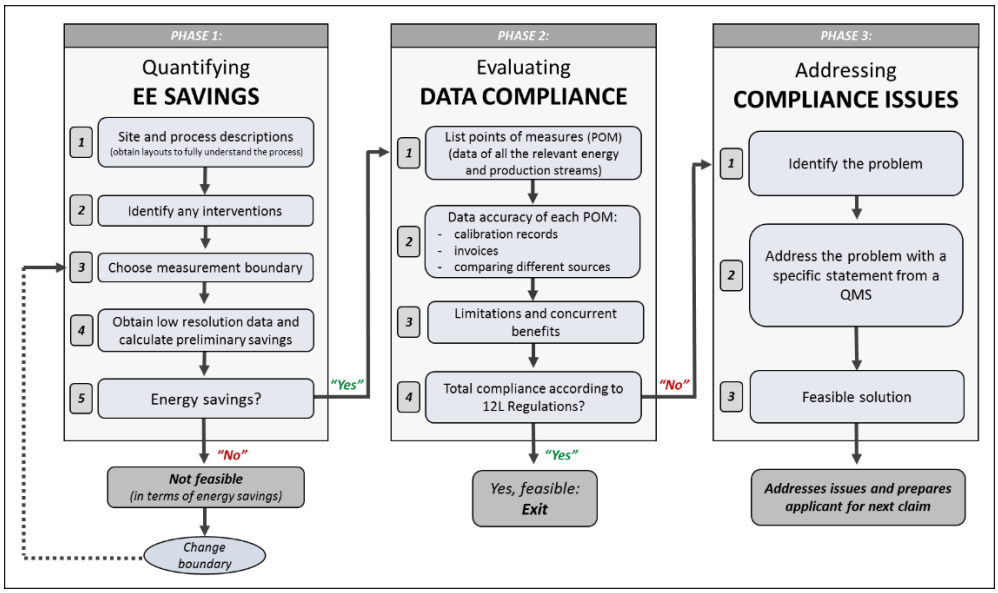


Figure 7: Strategy for evaluating 12L feasibility in energy-intensive industries

This strategy provides a way to simplify the process of a 12L feasibility investigation. It can provide the 12L applicant with practical guidelines to quantify potential, evaluate compliance, and address identified problems.

4 RESULTS

4.1 Case study

The final strategy is applied to various case studies, and is used to highlight specific scenarios or outcomes of the method. This case study represents the investigation for 12L feasibility in an underground gold mine. The investigation was done by implementing the strategy.

4.1.1 PHASE 1: Calculating EE savings

Electricity is the sole energy source used in underground mining. It is used by various sub-systems within the mine, such as fans, pumps, and other electricity-dependent systems within the shafts. Once the basic process is understood, *interventions* or energy savings measures must be *identified*, so that it is clear where the EE savings will occur.

It is known that several energy savings measures were implemented on the compressed air sub-systems. Due to these measures, the initial *measurement boundary* will isolate the compressed air system. This is shown below in Figure 8.

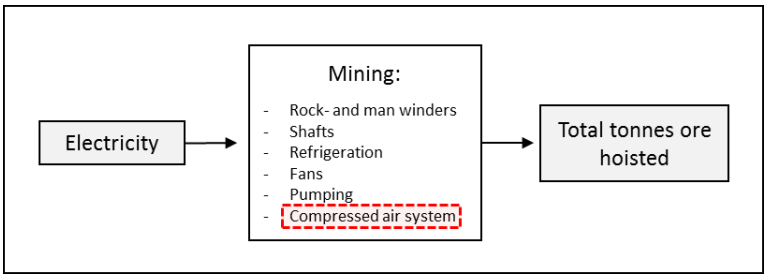


Figure 8: Case study — Initial measurement boundary

The next step requires *low-resolution data* for this specific boundary. The data obtained included monthly resolution electricity data as well as the total mass of ore hoisted from the mine. This is done in order to develop a baseline model that will be used to *calculate the preliminary EE savings*.

The *preliminary EE savings* can now be determined using two different calculation methods — i.e., an intensity calculation and a regression model. Figure 9 shows the monthly energy intensity of the gold mine's compressed air sub-system in kWh per tonne of ore hoisted.

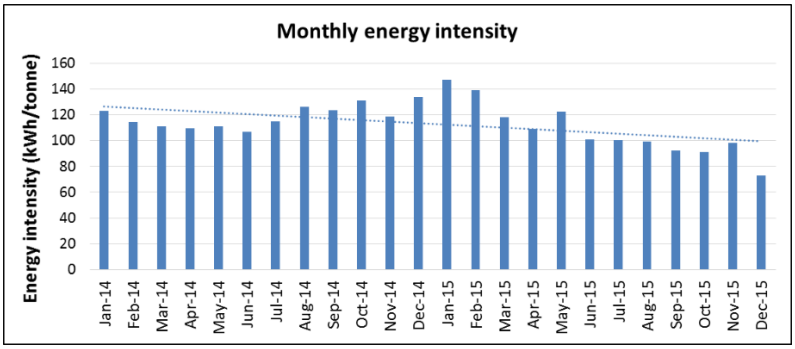


Figure 9: Case study — Monthly energy intensity

Improved energy efficiency can be observed from the baseline to the assessment year. Thus savings were achieved. The calculations are based on Equations 2, 3, 4; a summary is provided in Table 3.

Table 3: Case study — EE savings results (intensity calculation)

Energy intensity results summary		
Description	**2014**	**2015**
Total annual energy consumption (kWh)	400 282 443	345 603 013
Total annual production (tonnes)	3 401 911	3 284 825
Energy intensity (kWh/tonne)	118	105
Predicted energy (kWh)	386 505 636	345 603 013
Total annual energy savings (kWh)	**40 902 623**	

The intensity analysis showed an EE saving of 40.9 GWh. A regression model analysis will also be used to calculate EE savings, and is defined in Figure 10.

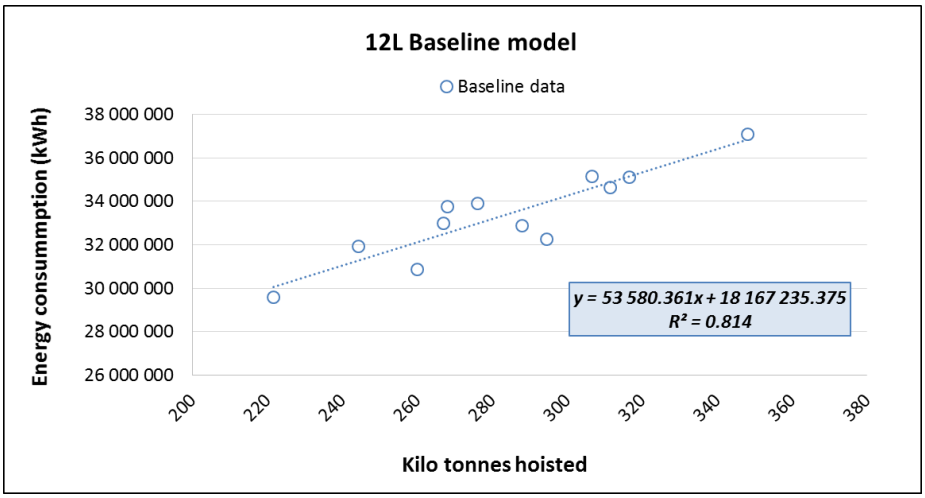


Figure 10: Case study — Baseline model

The statistical parameters (*m* and *c*) of the linear regression line are used to determine the predicted energy. This predicted, or adjusted, energy is plotted together with the actual energy in the figure below (Figure 11). This shows what the energy consumption would have been (red dashed line) if the system still operated under the same conditions as in the baseline period.

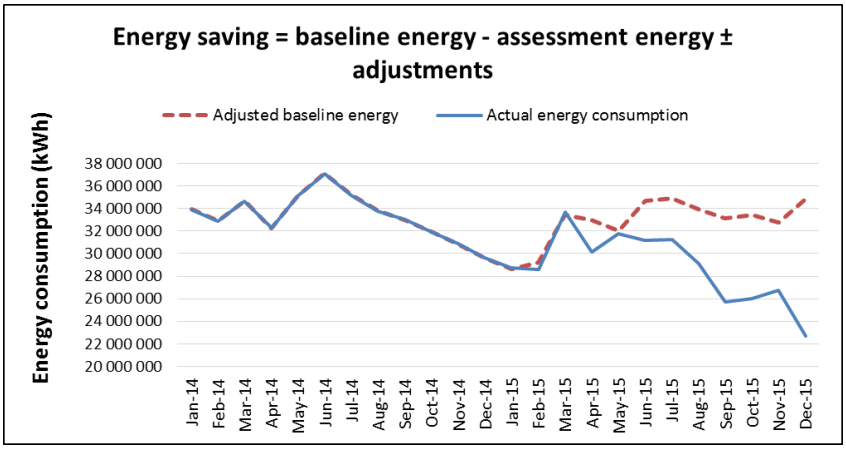


Figure 11: Case study — Actual vs adjusted energy

By using Equations 1 and 5, the regression analysis yielded positive EE savings. The results are summarised in Table 4.

Table 4: Case study — EE savings results (regression analysis)

Regression analysis results summary	
Actual assessment energy (kWh)	345 603 013
Predicted assessment energy (kWh)	394 008 933
Savings from baseline (kWh)	**48 405 920**

A visual representation of the results is given in Figure 12, where the EE savings results obtained through intensity and regression calculations are compared.

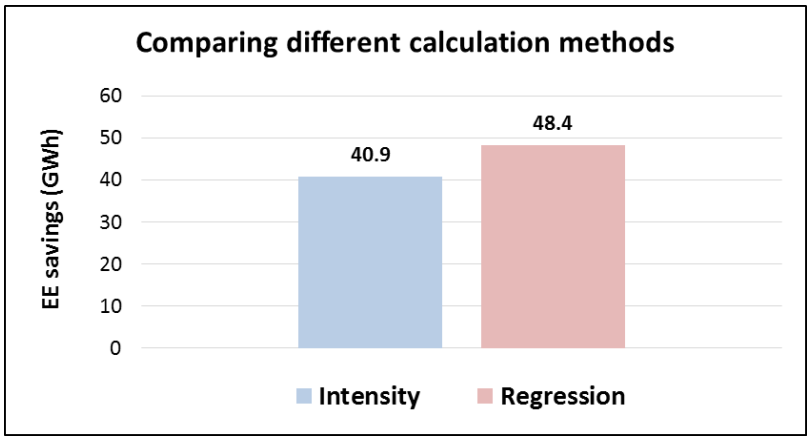


Figure 12: Case study — EE savings results (intensity vs regression analysis)

Since the EE savings are significant regardless of the method used (intensity = 40.9 GWh; regression = 48.4 GWh), the next phase may begin — i.e., *evaluating compliance*. This will be discussed in the next section.

4.1.2 PHASE 2: Evaluating compliance

Having an accurate and transparent 12L application is crucial. In order to confirm that the data (used to construct the baseline and assessment data sets) is in fact accurate, it must be critically assessed to ensure *compliance with the SANS 50010 Standard and 12L Regulations*.

The first step is to list all the energy streams and drivers entering and exiting the measurement boundary, together with their corresponding POM. Figure 13 provides a diagram of the POM within the chosen boundary (note the red meters, which indicate a lack of compliance).

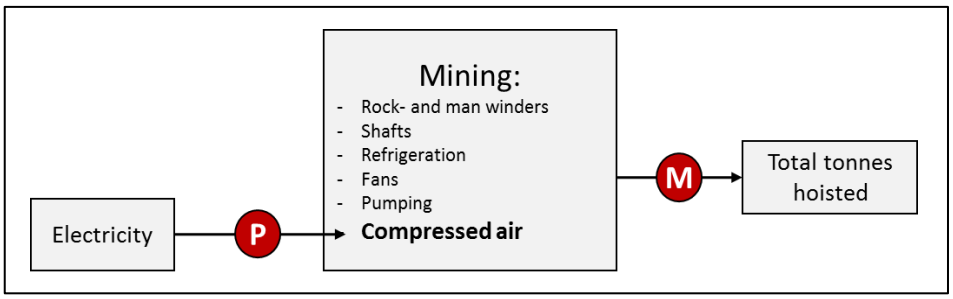


Figure 13: Case study — Measurement points

The list of energy carriers and drivers, together with their corresponding POM, includes the following (Table 5):

Table 5: Case study — List of measurement points

	Energy carrier / driver	*Point of measure*	*Measurement*	*Measuring device*	*Unit*
Energy carrier	Electricity	Power measurement (P)	Power	Power meter	kW
Energy driver	Tonnes hoisted	Mass measurement (M)	Tonnes hoisted	Scale	Tonnes

The compliance of the data of each POM must be evaluated by proving the ***accuracy*** of the data. This can be done through calibration records, invoices, or other certified reports or documentation. Unfortunately no calibrations, invoices, or other forms of proof for any of the data sets could be obtained; thus no 12L compliance could be proven. It was therefore necessary to proceed to the next phase, *addressing compliance issues*.

(However, if full 12L compliance could have been proven, and no concurrent benefits or limitations were applicable, the 12L potential on this specific energy-intensive industry would indeed have been feasible. The first and second steps (*determining EE savings; evaluating data compliance*) of the strategy could then have been completed, due to significant savings as well as compliant data.)

4.1.3 PHASE 3: Addressing compliance issues

The lack of data compliance during a 12L analysis may be one of the reasons for unsuccessful investigations. In the event of having issues with compliance, the 12L applicant must proceed to the next phase — *addressing compliance issues*. This step will aim to address the specific compliance issues using a quality management system.

In this case study, no 12L compliance could be proven, as no form of proof (the red meters in the process layout in Figure 13) for any of the data sets or data meters could be obtained. The quality of the measurement of the data is therefore considered untrustworthy. The issues of *data measurement* must therefore be addressed.

The involved meters or sensors should not only give accurate measurements: the data itself must be a true reflection of reality. Since the data sets of this case study could not be sufficiently verified to ensure the accuracy of the data, the issue of *data verification* must be addressed.

Several international standards or ISOs (International Organization for Standardization) address the issue of data measurement and verification. Table 6 (repeat of Table 2, with additional highlighted areas) indicates which QMSs are applicable to the specific issues identified.

Table 6: Addressing compliance issues with specific QMSs

	ISO 8000	ISO 9001	ISO 14001	ISO 50001	ISO 50010
Data measurement		X	X	X	X
Data traceability	X	X	X	X	
Data verification		X		X	
Data reporting				X	X

ISOs 9001, 14001, 50001 and 50010 are all applicable when addressing the specific compliance issues. The first, second, and third steps (*determining EE savings; evaluating data compliance; addressing compliance issues*) of the strategy could be implemented during the investigation of this case study, due to significant savings but non-compliant data.

4.2 Estimated benefit from additional case studies

As demonstrated in the case study, implementing the proposed strategy would provide the 12L applicant with the necessary guidelines for a practical application to evaluate the 12L feasibility of an energy-intensive industry.

An additional 47 cases were also investigated. Of the 47 investigations, 26 were successful in achieving EE savings. This translates to about 55 per cent of the evaluated industries managing to achieve EE savings. However, only four of the 26 successful investigations showing EE savings had data that complied with the 12L Regulations and Standard. This means that (in this case) more than 80 per cent of the energy-intensive industries did not have sufficient data management strategies in place.

Generic equations were developed to quantify the estimated benefit of using the proposed strategy. The cost benefit (Equation 6) and time benefit (Equation 7 and 8) can be aggregated to quantify the total financial benefit of implementing this strategy (assuming that it takes about 40 man-hours to complete a simple feasibility study, and 160 man-hours for a detailed investigation and for submitting the application to M&V and SANEDI):

Cost benefit (R):

$$Cost\ benefit\ (R) = (s - f) \times M\&V_{cost} \qquad \textit{(Equation 6)}$$

Time benefit (hours):

$$Time\ benefit\ (hours) = (a \times 160) - \{(f \times 160) + ((a - f) \times 40)\}$$
$$Time\ benefit\ (hours) = 160a - 160f - 40a + 40f$$
$$Time\ benefit\ (hours) = 120(a - f) \quad \textit{(Equation 7)}$$

Time benefit (R):

$$\frac{hours}{year} = 220\ \frac{working\ days}{year} \times 8 \frac{working\ hours}{day} = 1760\ \left(\frac{hours}{year}\right)$$
$$Time\ benefit\ (R) = \left[\frac{120(a-f)}{1760\ (\frac{hours}{year})}\right] \times Salary_{ann} \quad \textit{(Equation 8)}$$

where a = number of total investigations, f = number of feasible investigations, s = number of feasible investigations that comply with 12L Regulations, *M&V cost* = average cost of M&V (assumed to be R100 000 – R1 000 000 [29]), and $Salary_{ann}$ = average annual engineering salary (assumed to be R500 000 [30]).

By implementing the strategy and applying these formulas to the 47 additional case studies, it would appear that a cost and time benefit exceeding R2 200 000 and 5 160 man-hours respectively could have been obtained.

5 CONCLUSION

This study introduced a new strategy that could be followed throughout the process of investigating the feasibility of claiming the 12L tax incentive. This strategy would provide the 12L applicant with a holistic approach to conducting an initial internal investigation, before any unnecessary expense or time was wasted, when applying for the 12L tax incentive.

The results revealed that, by implementing the proposed strategy, the complexity of the 12L investigation decreases significantly. The results were then validated by quantifying the cost and time benefits of implementing the strategy, and resulted in significant savings.

REFERENCES

[1] **Davidson, O., Winkler, H., Kenny, A., Prasad, G., Nkomo, J., Sparks, D., Howells, M. & Alfstad, T.** 2006. *Energy policies for sustainable development in South Africa*. Cape Town: Energy Research Centre, University of Cape Town.

[2] **Republic of South Africa.** 2013. *Integrated planning report*. Pretoria: Department of Energy.

[3] **Republic of South Africa.** 2015. *12L Regulations in relation to the National Energy Efficiency Strategy*. Pretoria: Department of Energy.

[4] **Manuel, T.A.** 2009. *Republic of South Africa budget speech*. Pretoria: FormeSet Printers Cape (Pty) Ltd.

[5] **Du Toit, E.F.** 2011. *Energy efficiency savings allowance in South Africa: An international comparison*. Pretoria: University of Pretoria.

[6] **Steyn, K.** 2015. *EE Publishers - Section 12L tax allowance: Why the delay?* http://www.ee.co.za/article/section-12l-tax-allowance-delay.html [accessed 25/08/16].

[7] **Steyn, K.** 2014. *M&V Standard for 12L tax incentives*. Pretoria: SABS.

[8] **Republic of South Africa.** 2012. *Taxation Laws Amendment Act*. Pretoria: Government Gazette No. 36122.

[9] **National Treasury.** 2013. Regulations in terms of section 12L of the Income Tax Act, 1962, on the allowance for energy efficiency savings. Pretoria: Government Gazette No. 37136.

[10] **South African National Standard**. 2011. *SANS 50010:2011 Measurement and verification of energy savings*. Pretoria: SABS Standards Division.

[11] **GreenCape.** 2015. *12L income tax allowance on energy efficiency savings*. Cape Town: GreenCape.

[12] **SANAS.** 2015. *South African National Accreditation System*. http://home.sanas.co.za/?page_id=38 [accessed 13/10/16].

[13] **Campbell, K.** 2017. *Evaluating the feasibility of the 12L tax incentive for energy intensive industries*. Potchefstroom: North-West University.

[14] **IIBA.** 2006. *A guide to business analysis body of knowledge (BABOK)*, version 1.6. Toronto: International Institute of Business Analysis.

[15] **Davis, B., Lockwood, A., Alcott, P. & Pantelidis, I.** 2012. *Food and beverage management*. New York: Routledge Taylor & Francis Group.

[16] **Campbell, G.M. & Baker, S.** 2010. *Project goals for project managers*. Indianapolis: Alpha Books.

[17] **Schiefer, U. & Döbel, R.** 2001. *Mapa-project: A practical guide to integrated project planning and evaluation*. Budapest: Open Society Institute.

[18] **El-Sharkawy, A.** 2005. *Economic feasibility studies*. Cairo: Center for Advancement of Postgraduate Studies and Research in Engineering Sciences (CAPSCU), Faculty of Engineering, Cairo University.

[19] **Nykiel, R.A.** 2007. *Handbook of marketing research methodologies for hospitality and tourism*. Binghamton, NY: Haworth Press, Inc.
[20] **Bridgewater Management Consulting Group**. 2014. *Guide to preparing a feasibility study*. Thimblesofplenty.
[21] **Department of Information Resources.** 1992. *How to conduct a feasibility study*. Austin: DIANE Publishing Company.
[22] **Panneerselvam, R. & Senthilkumar, P.** 2009. *Project management*. New Delhi: PHI Learning Private Ltd.
[23] **IPMVP.** 2009. *International performance measurement & verification protocol*. Springfield: US Department of Energy.
[24] **International Standard.** 2008. *ISO 9001: Quality management systems*. Switzerland: ISO.
[25] **International Standard.** 2004. *ISO 14001: Environmental management systems*. Switzerland: ISO.
[26] **International Standard.** 2011. *ISO 50001: Energy management systems*. Switzerland: ISO.
[27] **International Organization for Standardization**. *ISO 8000*. http://www.iso.org/iso/home/search.htm?qt=8000&sort=rel&type=simple&published=on [accessed 18/05/16].
[28] **Green times. 2013.** *Claiming energy efficiency tax incentives*. http://thegreentimes.co.za/claiming-energy-efficiency-tax-incentives/ [accessed 25/08/16].
[29] **Department of Energy**. 2016. Draft post–2015 national energy efficiency strategy. *Government Gazette* No. 40515, Pretoria.
[30] **Mybroadband.** 2016. *Engineering salaries in South Africa*. http://mybroadband.co.za/news/business/160658-2016-engineering-salaries-in-south-africa.html [accessed 13/10/16].

SAIIE29 Proceedings, 24th – 26th of October 2018, Spier, Stellenbosch, South Africa © 2018 SAIIE

USING DATA-DRIVEN ANALYTICS TO DEVELOP A MATERIAL BALANCE OVER A FERROCHROME FURNACE

K. Campbell[1], W. Booysen[2] & M. Kleingeld[3]

[1]North-West University, CRCED-Pretoria, Pretoria, South Africa
kcampbell@rems2.com
[2]North-West University, CRCED-Pretoria, Pretoria, South Africa
wbooysen@rems2.com
[3]North-West University, CRCED-Pretoria, Pretoria, South Africa
mkleingeld@rems2.com

ABSTRACT

Furnaces used for ferrochrome production are complex systems. There are a significant number of inlet and outlet streams with various parameters. However, some of these parameters are not always measured, which can limit decision-making abilities. Linking available data and additional information together with data analytics can possibly produce estimates of the unknown streams. It is, therefore, necessary to perform a material balance on a typical ferrochrome furnace to evaluate the underlying fundamentals of this concept.
This paper provides a brief overview of the furnace parameters measured in practice, before presenting an approach to perform the material balance. The available measurements of input and output streams are used together with literature-based compositions. This analytical approach links the known composition together with the known mass to estimate the unknown streams. The analytics are structured in such a way that it can later be automated.

The approach is applied to several industrial case studies and the results are presented in order to provide a proof of concept. The analysis manages to balance all elements (in and out) within an accuracy margin of 1.25%. The results are further discussed to illustrate the potential benefit in various application areas.

This work was sponsored by ETA operations

[1] Ms. K. Campbell holds a Master's of Engineering in Mechanical Engineering from the North-West University. She is currently enrolled for a PhD degree at the North-West University's Centre for Research and Continued Engineering Development (CRCED) in Pretoria.

[2] Dr. W. Booysen is a registered professional engineer and holds a PhD in Electrical Engineering from the North-West University. He is currently a post-doctoral student at the North-West University's Centre for Research and Continued Engineering Development (CRCED) in Pretoria.

[3] Prof. M. Kleingeld is a registered professional engineer and holds a PhD in Mechanical Engineering. He is currently a lecturer at the North-West University's Centre for Research and Continued Engineering Development (CRCED) in Pretoria.

1. INTRODUCTION

Furnaces used for ferrochrome (FeCr) production are complex systems [1]. There are a significant number of inlet and outlet streams with various parameters [2]. However, due to difficulty (and in some cases financial restraints), some of these parameters are not always measured [3] which can limit decision-making abilities. Linking available data and additional information together with data analytics can possibly produce accurate estimates of the unknown streams. It is, therefore, necessary to perform a material balance on a typical ferrochrome furnace to evaluate the underlying fundamentals of this concept.

Section 2 of this paper will focus on research done on the FeCr production process as well as mass and composition measurements typically conducted at a furnace. Data quality analysis was also researched and summarised. The method to be followed for conducting a material balance over a typical FeCr furnace is described in Section 3. Even though every furnace is unique, generic steps and examples are provided. The methodology from Section 3 was applied to a real-life FeCr furnace and used as case study for this investigation. The results are provided and discussed in Section 4, while the paper is concluded in Section 5.

2. RESEARCH BACKGROUND

2.1 Ferrochrome production process

The process of FeCr production is an energy intensive one [4, 5]. The total electricity consumption of such a process typically ranges between 3.3 and 4.2 kWh/t of FeCr produced [6, 7, 8]. FeCr is mainly used for stainless steel production, where approximately 1 tonne is needed to produce 3 – 3.5 tonnes of stainless steel [9].

Production is accomplished by feeding raw materials in the form of chromite ores, carbon-rich materials (reductant such as anthracite, char, and coke), and additives (fluxes, in the form of quartz, limestone, dolomite, etc.) to an arc furnace [10, 11, 12]. In some cases, the raw materials are prepared before being fed to the furnace: pelletising, sintering, and drying techniques are often performed on raw materials to produce a dry and uniform feed to the furnace, which would increase furnace stability [13, 14].

Electricity is used to heat up the furnace and melt the raw materials by means of an electric arc [15, 16]. Due to the heat provided, various chemical reactions take place, causing reduction of the metal oxides within the chromite ore to a final metal product, FeCr. Together with the main metal product, waste material (slag) as well as off-gas also exit the furnace as by-products [17]. Figure 2-1 shows an illustration of this process [18].

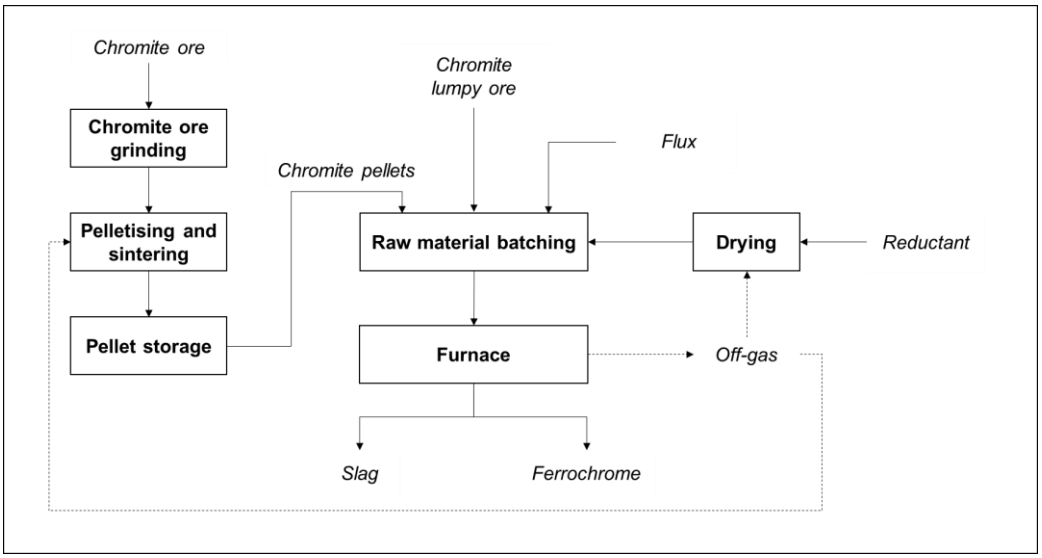


Figure 2-1: Ferrochrome production process

For the purpose of simplification, this diagram has been summarised to establish the focus area of this study: FeCr furnace, input, and output streams. A simplified illustration of this process is thus shown in the diagram below (Figure 2-2).

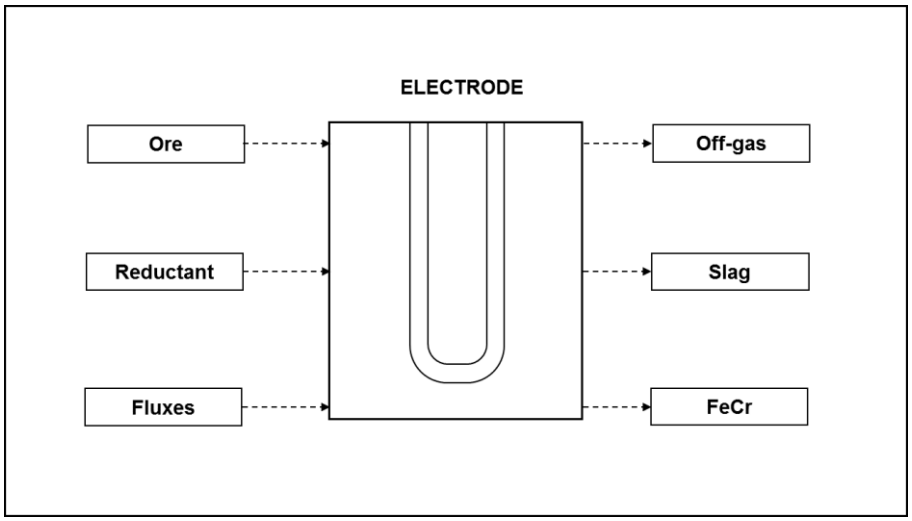


Figure 2-2: Simplified illustration of the FeCr production process

As mentioned, various reactions take place within the furnace which cause the FeCr product to be formed. The most significant reactions included the following [1, 18, 17, 19]:

$Cr_2O_3 + 3C \rightarrow 2Cr + 3CO$ Equation 2-1

$FeO + C \rightarrow Fe + CO$ Equation 2-2

$SiO_2 + 2C \rightarrow Si + 2CO$ Equation 2-3

$H_2O + C \rightarrow H_2 + CO$ Equation 2-4

$CO_2 + C \rightarrow 2CO$ Equation 2-5

$CaCO_3 \rightarrow CaO + CO_2$ Equation 2-6

From these reactions it can be assumed that the prominent elements present within the FeCr furnace are the following: Cr, Fe, C, Si, O, H, and Ca.

2.2 Typical measurements

Not all parameters are always measured at ferroalloy furnaces [20]. Mass balances can be used to predict mass and compositions of certain unmeasured streams [14]. The measurements typically available for the general furnace will be discussed briefly.

FeCr metal product

The main objective of the process referred to within this study is the production of FeCr metal, with a certain alloy grade. The mass and composition of the metal produced is therefore monitored closely and measured continuously [20]. The metal is tapped a few times per day, solidified, crushed, and then weighed on weigh-bridges[i]. Metal samples are also sent for regular (usually daily) composition analysis. A typical composition of FeCr product is as follows: 56.7% Cr, 33.8% Fe, 7.2% C, and 2.3% Si [21].

Raw materials

The mass of raw materials (chromite ore, reductant, and fluxes) are usually measured at weigh bins before being batched to the furnace [22]. The composition, however, is rarely known on site. Occasionally sampling of the reductants takes place on site. However, this is generally done long before batching (before materials are stored on stockpiles) creating a significant buffer capacity. From literature, the composition of each of the raw materials normally used in FeCr production is summarised below:

Cr ore: 50% Cr_2O_3, 25% FeO, 9% MgO, 10% Al_2O_3, 5% SiO_2, 1% CaO [21]

Anthracite: 88.94% C, 3.4% H, 2.32% O, 1.55% N, 0.8% S [23]

Char: 77.84% C, 0.34% H, 21.11% O, 0.71% N [24]

Coke: 89% C, 3.6% H, 1.56% H, 4.95% S [25]

Dolomite: 100% $CaMg(CO_3)_2$ [26]

Limestone: 100% $CaCO_3$ [27]

Quartz: 100% SiO_2 [28]

By-products

The two by-products (slag and off-gas) have often been considered waste streams and are rarely measured accurately[ii]. The slag composition is, however, estimated to ensure the required slag composition [29]. From time to time, the slag mass is calculated by using a slag to metal ratio (usually between 1.1 and 1.8 tonnes of slag produced per tonnes of metal [30]), which is estimated by random sampling. The amount of slag produced can also be estimated based on an aluminium (Al_2O_3) balance. This is done with the assumption that the slag analysis is done accurately and representatively [31].

Then slag and off-gas compositions are given below:

Slag: 23.2% SiO_2, 24.7% Al_2O_3, 19.8% MgO, 3.0% CaO, 10.7% FeO, 18.6% Cr_2O_3 [31]

Off-gas: 75-90% CO, 2-10% CO_2, 2-15% H_2, 2-7% N_2 [2, 19]

The typical compositions are converted to element-based compositions by using the molecular weight of each formula and element. The results are summarised in Table 2-1:

Table 2-1: Typical compositions for streams entering and exiting a FeCr furnace (element-based)

	Fe	Cr	Si	S	C	Al	O	Ca	Mg	H	N
A	17.5	34.2	2.3	-	-	5.2	34.6	0.7	5.4	-	-
B	-	-	-	0.8	88.9	-	2.3	-	-	3.4	1.6
C	-	-	-	-	77.8	-	21.1	-	-	0.3	0.7
D	-	-	-	5.0	89.0	-	0	-	-	3.6	1.6
E	-	-	-	-	13.0	-	52.2	21.7	13.0	-	-
F	-	-	-	-	12.0	-	48.0	40.0	-	-	-
G	-	-	46.7	-	-	-	53	-	-	-	-
H	33.8	56.7	2.3	-	7.2	-	-	-	-	-	-
I	8.3	12.7	10.8	-	-	12.8	41.3	2.1	11.9	-	-
J	-	-	-	-	33-41	-	45-59	-	-	2-15	2-7

** Chrome ore = A, anthracite = B, char = C, coke = D, dolomite = E, limestone = F, quartz = G, FeCr metal = H, slag = I, off-gas = J.*

The typical mass ratio of input and output streams are as follows [17, 18]:

- 2.1 – 2.4 tonnes Cr ore fed per tonne FeCr metal produced
- 0.5 – 0.55 tonnes reductants fed per tonne FeCr metal produced
- 0.1 – 0.45 tonnes fluxes per tonne FeCr metal produced
- 1.1 – 1.3 tonnes slag per tonne FeCr metal produced
- 0.9 – 1.1 tonnes off-gas per tonne FeCr metal produced

The chromium recovery of this process is usually around 80% - 85% [18].

2.3 Data quality

Data quality is an important factor for a number of reasons and needs to be monitored pro-actively [32]. When evaluating a FeCr furnace, a significant amount of data needs to be collected, processed, and analysed. Therefore, thorough data evaluation is necessary.

A study done by Booysen [33] provided a data quality evaluation method that was developed to identify any potential errors and abnormalities. This method consists of four steps: the first three steps aim to identify abnormal measurements, whereas the final step identifies abnormal operation. A schematic flow of this method is shown in Figure 2-3.

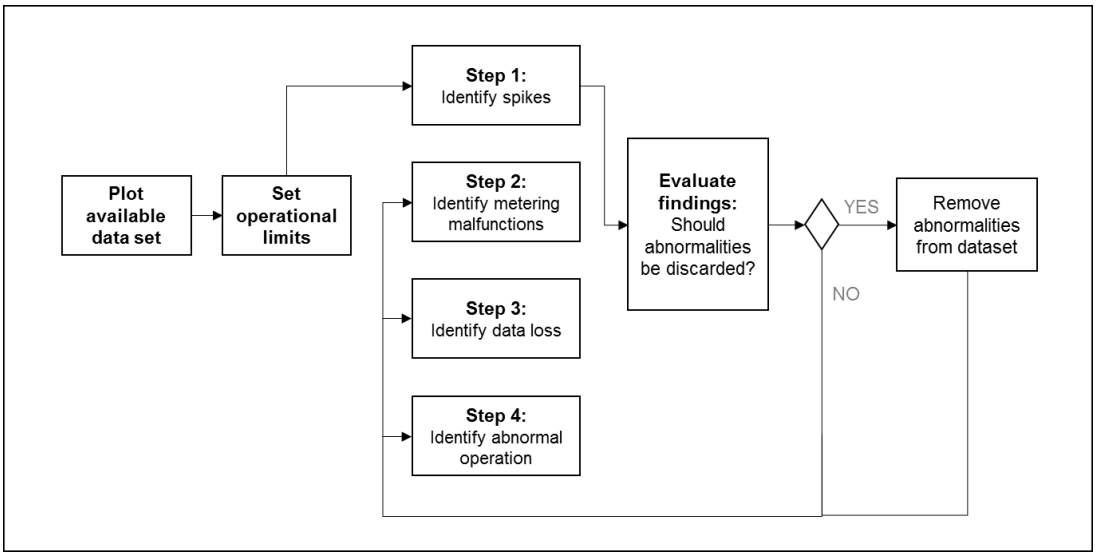


Figure 2-3: Data quality evaluation [33]

Figure 2-4 provides a simplified visualisation of a dataset containing typical measurement abnormalities. The minimum and maximum limits are selected based on the variable being assessed. Steps 1 – 3 are indicated on this figure as follows: data spikes (step 1), faulty data (step 2), and data loss (step 3).

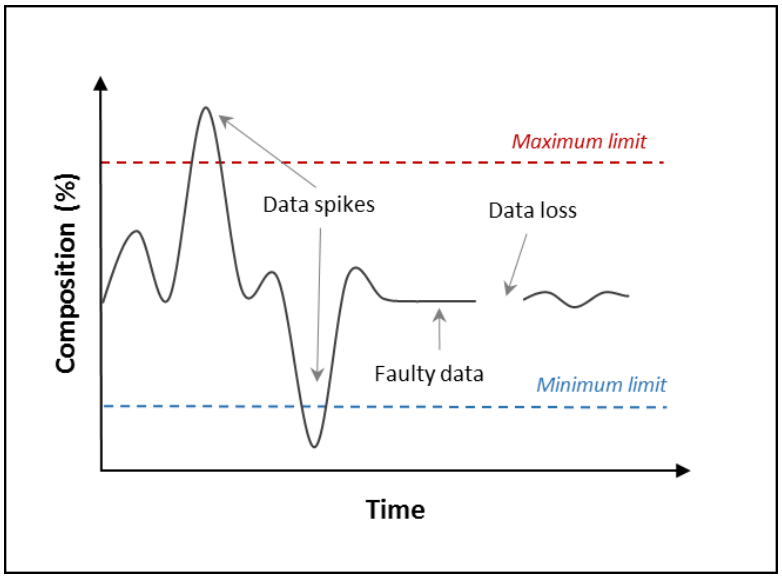


Figure 2-4: Data evaluation – Identifying abnormal measurements

The first step of identifying abnormal measurements within the data evaluation method, aims to detect data spikes. Data spikes happen when there is a failure on measurement equipment or when communication is briefly lost. Even though these tend to happen over short periods of time, their amplitude (very high or very low) can still significantly influence the accuracy of calculations.

The next step is to identify metering malfunctions, which could lead to faulty data being logged. This occurrence is illustrated as a constant value in Figure 2-4, where the last data reading is typically repeated for a number of resolutions, until the malfunction has been resolved. Even though this data will still fall within the operational limits, the results will be influenced by this incorrect, constant value.

Step 3 aims to identify data loss. This can generally be detected where no data has been recorded, as indicated by the blank space in Figure 2-4. The final step of this method aims to identify abnormal system operation. This is illustrated by Figure 2-5.

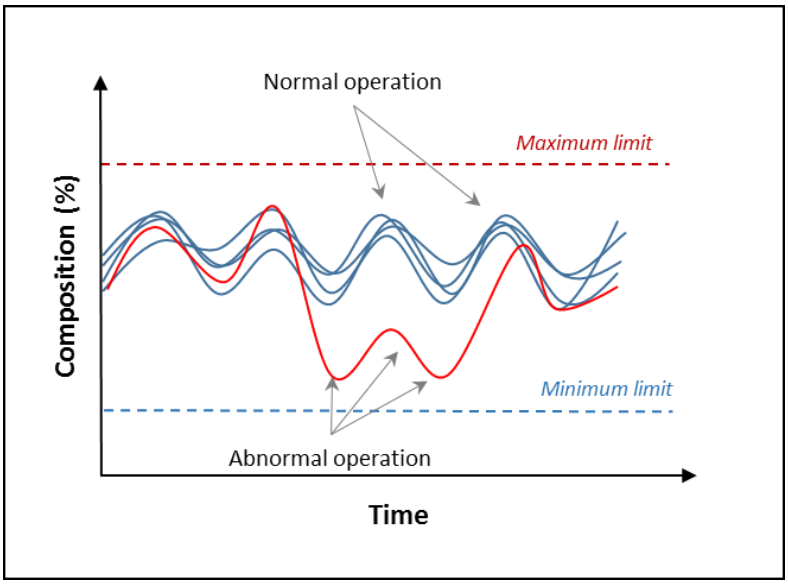


Figure 2-5: Data evaluation – Identifying abnormal operation

In Figure 2-5 there are numerous profiles that follow the same trend, indicating normal operation. The red profile however is deemed abnormal, as it differs from the trend. The utmost care should be taken when investigating these results as there is, unfortunately, no fixed rule as to what is defined as “abnormal operation”. This step therefore requires a thorough understanding of the process being evaluated.

The aim of this data quality evaluation method is to evaluate a dataset, remove any measurement abnormalities, and identify operational abnormalities. An accurate, high quality dataset is the final outcome of this method.

2.4 Research background conclusion

The research background section focused on the following:

- The basic process of FeCr production, so that all the theoretical components and elements are known to the reader.
- The typical setup and measurements, so that the reader can understand the practical implications and challenges faced when conducting a mass balance.
- Data quality, so that the practical data can be assessed to be usable before being included in the mass balance.

This was applied to develop a functional method on constructing a mass balance for a typical FeCr furnace.

3. METHODOLOGY

The methodology is divided into three main steps: *Collect information, layouts, and data*; *evaluate data quality*; and *construct a material balance*. An overview of this strategy is presented in Figure 3-1.

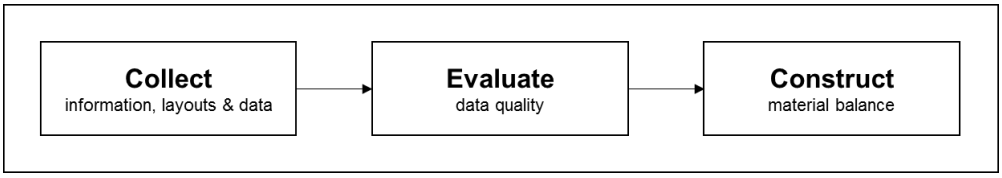
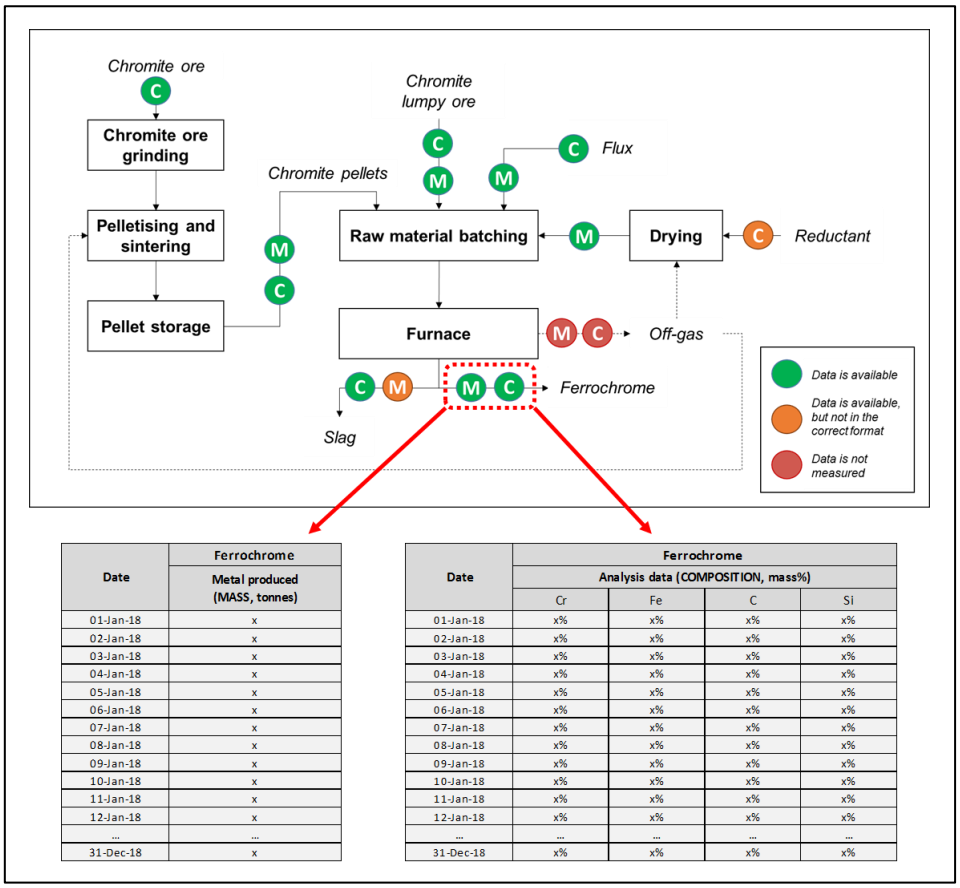


Figure 3-1: Basic three-step methodology for developing a FeCr material balance

This strategy provides the basic knowledge to developing a material balance, based on data-driven analytics. Each step is discussed in more detail in Sections 3.1 through 3.3.

3.1 Collect information, layouts, and data

The first step is to collect all relevant information from the site being evaluated. This includes layouts of the furnace, the relevant points of measurement indicated on layouts, as well as the corresponding mass and composition data for the evaluation period. Figure 3-2 indicates the outcome of this step. Note that for illustration purposes, only data collected for ferrochrome metal produced is shown on the layout (mass and composition data). However, data from all available streams must be collected.



Date	Ferrochrome
	Metal produced (MASS, tonnes)
01-Jan-18	x
02-Jan-18	x
03-Jan-18	x
04-Jan-18	x
05-Jan-18	x
06-Jan-18	x
07-Jan-18	x
08-Jan-18	x
09-Jan-18	x
10-Jan-18	x
11-Jan-18	x
12-Jan-18	x
...	...
31-Dec-18	x

Date	Ferrochrome			
	Analysis data (COMPOSITION, mass%)			
	Cr	Fe	C	Si
01-Jan-18	x%	x%	x%	x%
02-Jan-18	x%	x%	x%	x%
03-Jan-18	x%	x%	x%	x%
04-Jan-18	x%	x%	x%	x%
05-Jan-18	x%	x%	x%	x%
06-Jan-18	x%	x%	x%	x%
07-Jan-18	x%	x%	x%	x%
08-Jan-18	x%	x%	x%	x%
09-Jan-18	x%	x%	x%	x%
10-Jan-18	x%	x%	x%	x%
11-Jan-18	x%	x%	x%	x%
12-Jan-18	x%	x%	x%	x%
...	...	...	...	...
31-Dec-18	x%	x%	x%	x%

Figure 3-2: Collect information, layouts, and data

The circles on the layout represent points of (required) measure. Green circles indicate that data is available, the orange represent data available, however not in the correct format, while the red circles indicate that data is not available, or not even measured. The "M" symbols refer to mass measurements (by means of weighbridges or weigh bins), whereas the "C" denotes composition analysis sampling taking place.

If data is to be required for an orange-indicated measurement point (data that is available, but not in the correct format), data needs to be processed to the correct analysis by making use of various assumptions or methods. An example of such a case is when the reductant composition is based on proximate analyses instead of ultimate analyses. The slag mass may also not be available, however, slag to metal ratio data can be used to calculate a theoretical slag mass.

3.2 Evaluate data quality

Having an accurate and "good" quality dataset is essential. It is important that all the data received in step 1 is a reflection of the truth. Step 2 of the methodology is thus to evaluate the data quality.
The method provided in section 2.3 (Figure 2-3) needs to be followed for all mass and composition measurements in order to clean the dataset. This will ensure a representative, "good" quality dataset. Only then can the data be processed and used in further calculations.

3.3 Constructing a mass balance

A basic mass, or material balance is based on the principle of "mass in equals mass out" [34]. A material balance can be performed on the total mass entering and exiting the FeCr furnace, but also based on the individual chemical elements. These two different approaches are shown in Equation 3-1 and Equation 3-2, respectively:

$$M_{ore} + M_{reductant} + M_{flux} = M_{FeCr} + M_{slag} + M_{off-gas} \qquad \text{Equation 3-1}$$

$$\sum(M_{X_{in}}) = \sum(M_{X_{out}}) \qquad \text{Equation 3-2}$$

Where "M" represents the total mass of a certain stream or element, and "X" refers to a certain chemical element. Constructing a mass balance is the third and final step of the method, as referred to by Figure *3-1*. This step will however take place over four different phases:

3.3.1 Calculate total mass of unmeasured streams

From the research section in 2.2, it is gathered that the mass of all batching streams (ore, reductant, and flux) are generally measured, as well as the mass of FeCr produced. Slag mass data is usually in the form of a ratio; however, it can be derived to estimate the total mass of slag. Thus, the only unknown stream mass is that of off-gas. By using Equation 3-1, the mass of the total off-gas stream can be calculated.

3.3.2 Assume the composition of all streams

Section 2.2 was summarised into Table 2-1 which provided the typical compositions for streams entering and exiting a FeCr furnace (element-based). This table can be used to assign compositions to all material streams. Since the total mass of each input and output stream is known, the theoretical mass of each element entering and exiting the furnace can be calculated. This is illustrated in Table 3-1, where A_1 (lit) refers to the mass of element "1" present in stream "A" (based on literature composition).

Table 3-1: Mass per element based on literature compositions

Stream	**Mass per element** *(tonnes)*				
	1	2	3	…	x
A	A_1 (lit)	A_2 (lit)	A_3 (lit)	…	A_x (lit)
B	B_1 (lit)	B_2 (lit)	B_3 (lit)	…	B_x (lit)
C	C_1 (lit)	C_2 (lit)	C_3 (lit)	…	C_x (lit)
…	…	…	…	…	…
n	n_1 (lit)	n_2 (lit)	n_3 (lit)	…	n_x (lit)

3.3.3 Update the assumed compositions with measured plant data

After the literature compositions were used to assume the mass of each element, actual plant data can be used to replace the data from literature. For the purpose of this example, note that composition data for streams A and C was available. This is illustrated in Table 3-2, where "A_1 (lit)" was replaced by "A_1 (actual)".

Table 3-2: Mass per element updated with measured compositions (where applicable)

Stream	Mass per element *(tonnes)*				
	1	2	3	…	x
A	A_1 (actual)	A_2 (actual)	A_3 (actual)	…	A_x (actual)
B	B_1 (lit)	B_2 (lit)	B_3 (lit)	…	B_x (lit)
C	C_1 (actual)	C_2 (actual)	C_3 (actual)	…	C_x (actual)
…	…	…	…	…	…
n	n_1 (lit)	n_2 (lit)	n_3 (lit)	…	n_x (lit)

3.3.4 Visualising results

Once all streams are updated with actual plant data (where available), the results of the mass balance can be visualised in various different ways. An example of a desired plot is the total mass in vs. total mass out (based on Equation 3-2). This plot is shown in Figure 3-3:

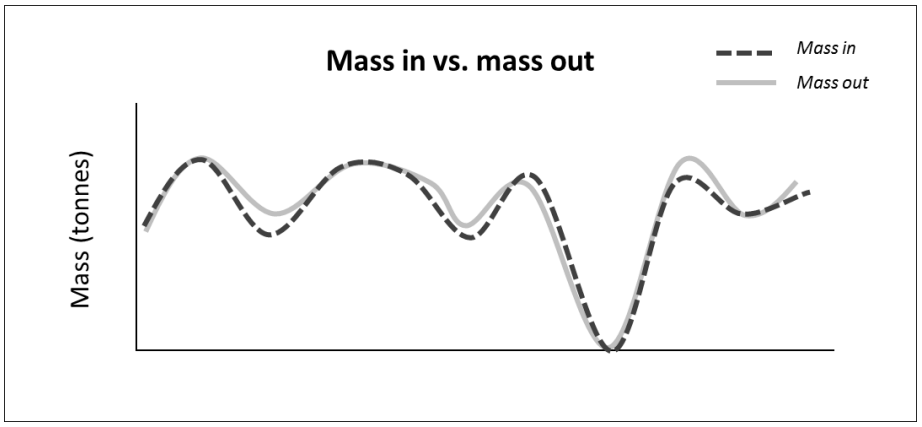


Figure 3-3: Visualising results

A final mass balance error can also be calculated by using the following equation:

$$Mass\ balance\ error\ (\%) = \frac{\Sigma\left(M_{X_{in}}\right) - \Sigma\left(M_{X_{out}}\right)}{\Sigma\left(M_{X_{in}}\right)} \qquad \text{Equation 3-3}$$

For the purpose of this study, an error margin of 3% has been chosen as an acceptable error.

3.4 Final methodology

The three steps (from section 3.1, 3.2 and 3.3) can be combined to present the final methodology to be followed for developing a material balance over a FeCr furnace (presented in Figure 3-4).

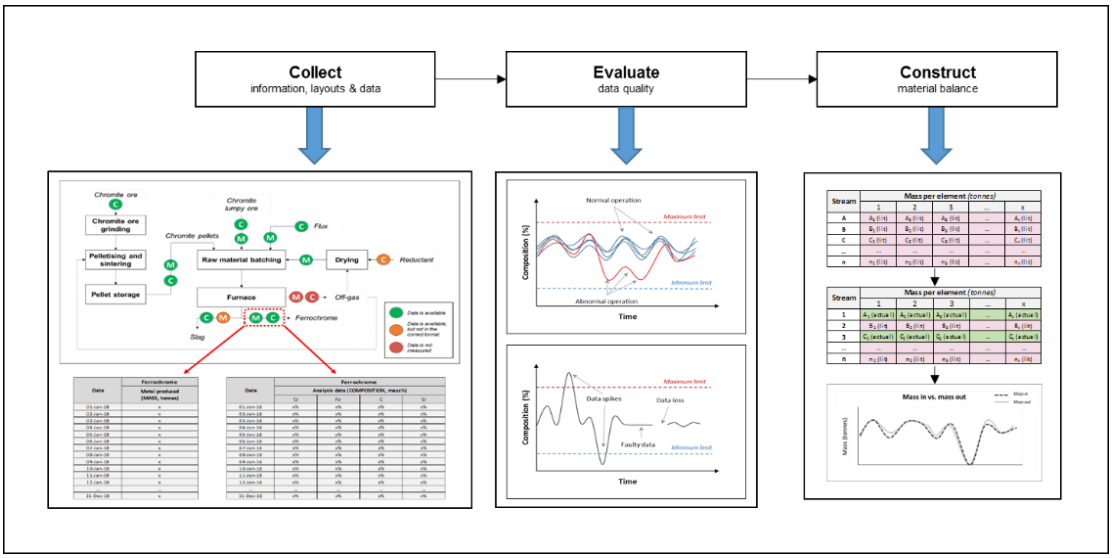


Figure 3-4: Final three-step methodology for developing a FeCr material balance

4. CASE STUDY: RESULTS AND DISCUSSION

The final methodology is applied to an industrial case study and is used to highlight the specific outcomes of the method.

4.1 Collect information, layouts, and data

Furnace X is evaluated in terms of the methodology. A layout of the furnace, the relevant points of measure as well as the corresponding mass and composition data over a three-year evaluation period has been collected. This is shown in Figure 4-1.

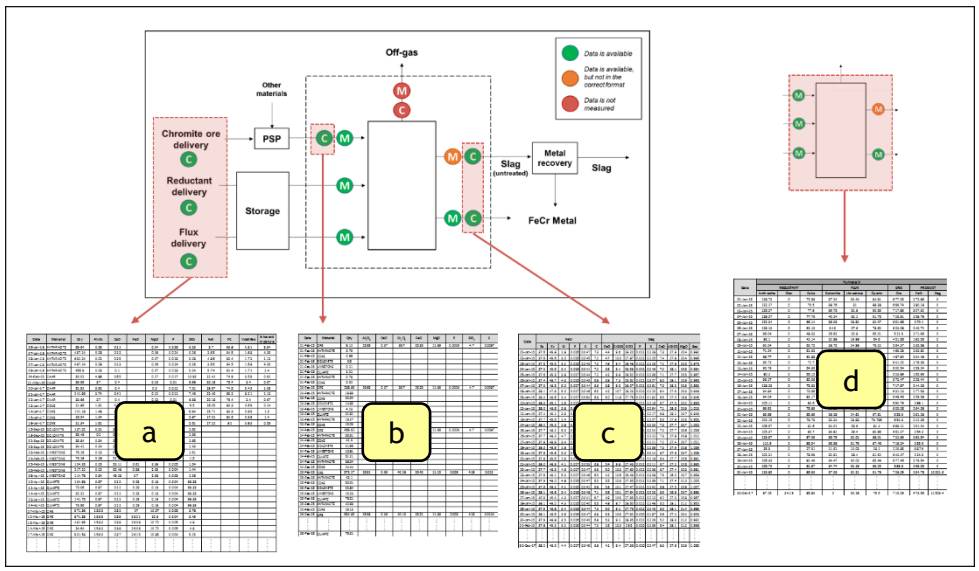


Figure 4-1: Collect information, layouts, and data

Chrome ore, reductant (anthracite, char, and coke), and fluxes (dolomite, limestone, and quartz) are sampled on delivery (dataset “a”). Chromite ore is pelletised (PSP), and sampled again before batching (dataset “b”).

The composition of the FeCr metal and slag is also determined when exiting the furnace (dataset "c"). The mass of all raw materials is determined in weigh bins right before batching, whereas the FeCr metal and slag mass are measured at weigh bridges (dataset "d").

These four datasets have been collected so as to be evaluated throughout the next step (4.2). Note that the slag mass meter is indicated in orange. This is due to the slag mass only being logged per month, when the rest of the data is in daily resolution. Thus, all data will be converted to monthly resolution when processing and calculations commence.

The time delay that may occur between mass and composition measurements is uncertain. All compositions will therefore be averaged to a constant annual value, in order to compensate for any possible storage capacities.

4.2 Evaluate data quality

The raw datasets as received in 4.1 (datasets "a", "b", "c", and "d") were evaluated based on the method discussed in Section 2.3. Figure 4-2 illustrates one of the datasets before and after the dataset has been cleaned.

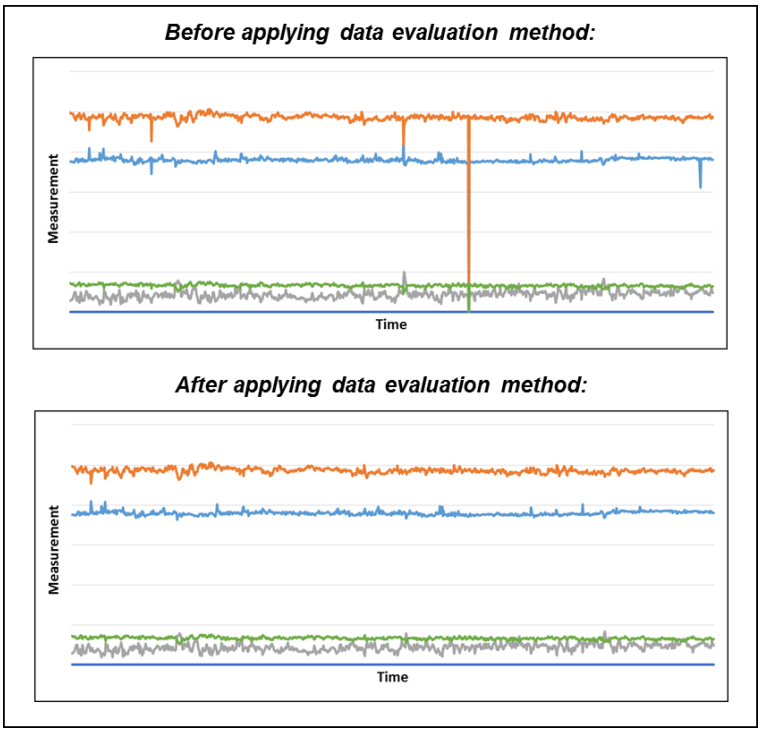


Figure 4-2: Data quality evaluation

Any abnormal measurements within the data have been identified, investigated, and removed if necessary. Annual shutdowns were detected (where furnace was shut down for a month or two), however data was not removed since this is not an abnormal operational occurrence. Consequently, after applying the method of data quality evaluation, all datasets are of high quality and can be used in the final step to construct a mass balance.

4.3 Constructing a mass balance

4.3.1 Calculate total mass of unmeasured streams

From Section 4.1 it was noted that the only unknown mass is that of the off-gas stream. By using Equation 3-1, the mass of the total off-gas stream can be calculated:

$$M_{ore} + M_{reductant} + M_{flux} = M_{FeCr} + M_{slag} + M_{off-gas}$$
$$M_{off-gas} = M_{ore} + M_{anth} + M_{char} + M_{coke} + M_{dolomite} + M_{limestone} + M_{quartz} - M_{FeCr} - M_{slag}$$

Table 4-1: Calculating the total mass of unmeasured (off-gas) streams

Date	Consumption							Production		
	REDUCTANT			FLUX			ORE	FeCr	Slag	Off-gas
	Anth.	Char	Coke	Dolomite	Limestone	Quartz	Ore			
Jan-15	x xxx	0	x xxx	xxx	xxx	x xxx	xx xxx	x xxx	xx xxx	x xxx
Feb-15	x xxx	0	x xxx	xxx	xxx	x xxx	xx xxx	x xxx	x xxx	x xxx
Mar-15	x xxx	0	x xxx	xxx	xxx	x xxx	xx xxx	x xxx	xx xxx	x xxx
Apr-15	x xxx	0	x xxx	xxx	xxx	x xxx	xx xxx	x xxx	xx xxx	x xxx
May-15	x xxx	0	x xxx	xxx	xxx	x xxx	xx xxx	x xxx	xx xxx	x xxx
Jun-15	0	0	0	0	0	0	0	0	0	0
Jul-15	0	0	0	0	0	0	0	0	0	0
Aug-15	xxx	0	xxx	xxx	0	xxx	x xxx	x xxx	x xxx	x xxx
Sep-15	x xxx	xxx	x xxx	xxx	0	x xxx	xx xxx	x xxx	xx xxx	x xxx
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
Dec-17	x xxx	xxx	x xxx	0	xxx	x xxx	xx xxx	x xxx	xx xxx	x xxx

Since all mass streams are now known, the next phase of constructing a mass balance can be investigated.

4.3.2 Assume the composition of all streams

Table 2-1 is used to assign compositions to all material streams. Since the total mass of each input and output stream is known, the theoretical mass of each element entering and exiting the furnace is calculated. This is illustrated in Table 4-2, where the pink blocks represent mass per element (calculated by using literature compositions).

Table 4-2: Mass per element based on literature compositions

Date	Anthracite					Char				Coke				Dolomite							Limestone						
	S	C	O	H	N	C	O	H	N	S	C	H	N	Fe	Si	C	Al	O	Ca	Mg	Fe	Si	C	Al	O	Ca	Mg
Jan-15	xx	xxxx	xx	xxx	xx	0	0	0	0	xxx	xxxx	xx	xx	0	0	xxx	0	xxx	xxx	xxx	0	0	xxx	0	xxx	xxx	0
Feb-15	xx	xxxx	xx	xx	xx	0	0	0	0	xx	xxxx	xx	xx	0	0	xx	0	xxx	xxx	xx	0	0	xx	0	xxx	xxx	0
Mar-15	xx	xxxx	xx	xxx	xx	0	0	0	0	xxx	xxxx	xx	xx	0	0	xxx	0	xxx	xxx	xxx	0	0	xxx	0	xxx	xxx	0
Apr-15	xx	xxxx	xx	xxx	xx	0	0	0	0	xx	xxxx	xx	xx	0	0	xx	0	xxx	xxx	xx	0	0	xxx	0	xxx	xxx	0
May-15	xx	xxxx	xx	xxx	xx	0	0	0	0	xxx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xx	0	xxx	xxx	0
Jun-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-15	xx	xxx	xx	xx	xx	0	0	0	0	xx	xxx	xx	x	0	0	xx	0	xxx	xx	xx	0	0	0	0	0	0	0
Sep-15	xx	xxxx	xx	xxx	xx	xxx	xx	x	x	xx	xxxx	xx	xx	0	0	xxx	0	xxx	xxx	xxx	0	0	0	0	0	0	0
Oct-15	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xx	xxxx	xx	xx	0	0	xxx	0	xxx	xxx	xxx	0	0	x	0	xx	xx	0
Nov-15	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xxx	xx	0	0	xx	0	xxx	xxx	0
Dec-15	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xx	0	xxx	xxx	0
Jan-16	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xxx	xx	0	0	xx	0	xx	xx	0
Feb-16	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xxx	xx	0	0	0	0	0	0	0
Mar-16	xx	xxxx	xx	xxx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xxx	0	xxx	xxx	0
Apr-16	xx	xxxx	xx	xx	xx	xxx	xx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xx	0	xxx	xxx	0
May-16	xx	xxxx	xx	xx	xx	xxx	xx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xx	0	xxx	xxx	0
Jun-16	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	xx	0	xxx	xxx	xx	0	0	xx	0	xxx	xxx	0
Jul-16	x	xxxx	xx	xx	xx	xxx	xx	x	x	xx	xxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xx	0	xxx	xxx	0
Aug-16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sep-16	xx	xxxx	xx	xx	xx	xxx	xx	x	x	xx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xx	0	xxx	xxx	0
Oct-16	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	xx	0	xxx	xx	xx	0	0	xxx	0	xxx	xxx	0
Nov-16	xx	xxxx	xx	xxx	xx	xx	x	0	0	xxx	xxxx	xx	xx	0	0	x	0	xx	x	x	0	0	xxx	0	xxx	xxx	0
Dec-16	xx	xxxx	xx	xxx	xx	xxx	xx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Jan-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Feb-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Mar-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Apr-17	xx	xxxx	xx	xx	xx	xxxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
May-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Jun-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Sep-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xx	0	xxx	xxx	0
Oct-17	xx	xxxx	xx	xxx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xxx	0	xxx	xxx	0
Nov-17	xx	xxxx	xx	xxx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xxx	0	xxx	xxx	0
Dec-17	xx	xxxx	xx	xx	xx	xxx	xxx	x	x	xxx	xxxx	xx	xx	0	0	0	0	0	0	0	0	0	xxx	0	xxx	xxx	0

Date	Quartz						Ore										FeCr				Slag									OFF-GAS			
	Fe	Si	Al	O	Ca	Mg	Fe	Cr	Si	P	S	C	Al	O	Ca	Mg	Fe	Cr	Si	C	Fe	Cr	Si	P	S	Al	O	Ca	Mg	C	O	H	N
Jan-15	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Feb-15	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
Mar-15	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Apr-15	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
May-15	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jun-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-15	0	xxx	0	xxx	0	0	xxx	xxxx	xxx	0	0	0	xxx	xxxx	xx	xxx	xxx	xxxx	xxx	xxx	xxx	xxx	xxx	0	0	xxx	xxx	xx	xxx	xxx	xxx	xxx	xxx
Sep-15	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Oct-15	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Nov-15	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Dec-15	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
Jan-16	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Feb-16	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Mar-16	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Apr-16	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
May-16	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jun-16	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jul-16	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xx
Aug-16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sep-16	0	xxx	0	xxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
Oct-16	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Nov-16	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Dec-16	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jan-17	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Feb-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Mar-17	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Apr-17	0	xxxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
May-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jun-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Sep-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Oct-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Nov-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Dec-17	0	xxx	0	xxxx	0	0	xxxx	xxxx	xxx	0	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxxx	xxxx	0	0	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx

4.3.3 Update the assumed compositions with measured plant data

Actual plant data can be used to replace the data used from literature. As indicated in Figure *4-1*, all streams' compositions are available, except for the off-gas. This is illustrated in Table *4-3*, where the pink blocks represent mass per element calculated by using literature compositions, and the green blocks represent mass per element calculated by using actual measured plant data.

Table 4-3: Mass per element updated with measured compositions (where applicable)

Date	ANTHRACITE					CHAR					COKE			DOLOMITE							LIMESTONE						
	S	C	O	H	N	C	O	H	N	S	C	H	N	Fe	Si	C	Al	O	Ca	Mg	Fe	Si	C	Al	O	Ca	Mg
Jan-15	0	xxxx	xxx	xxx	xx	0	0	0	0	0	xxxx	xx	xx	x	xx	xx	x	xxx	xxx	xxx	x	x	xx	x	xxx	xxx	xx
Feb-15	0	xxxx	xxx	xxx	xx	0	0	0	0	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xxx	x	x	xx	x	xxx	xxx	xx
Mar-15	0	xxxx	xxx	xxx	xx	0	0	0	0	0	xxxx	xx	xx	x	xx	xx	x	xxx	xxx	xxx	x	x	xx	x	xxx	xxx	xx
Apr-15	0	xxxx	xxx	xxx	xx	0	0	0	0	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
May-15	0	xxxx	xxx	xxx	xx	0	0	0	0	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Jun-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-15	0	xxx	xxx	xx	xx	0	0	0	0	0	xxx	xx	xx	x	x	xx	0	xxx	xx	xx	0	0	0	0	0	0	0
Sep-15	0	xxxx	xxx	xx	xx	xxx	xx	xx	x	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xxx	0	0	0	0	0	0	0
Oct-15	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xxx	0	x	x	0	xx	xx	x
Nov-15	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xxx	x	x	xx	x	xxx	xxx	xx
Dec-15	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Jan-16	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xxx	x	x	x	x	xxx	xxx	x
Feb-16	0	xxxx	xxx	xx	xx	xxx	xxx	xx	x	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xxx	0	0	0	0	0	0	0
Mar-16	0	xxxx	xxx	xxx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Apr-16	0	xxxx	xxx	xx	xx	xxx	xx	x	x	0	xxxx	xx	xx	x	x	xx	x	xxx	xx	xx	x	x	xx	x	xxx	xxx	xx
May-16	0	xxxx	xxx	xx	xx	xxx	xx	x	x	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Jun-16	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Jul-16	0	xxx	xxx	xx	xx	xxx	xx	x	xx	0	xxx	xx	xx	x	x	xx	x	xx	xx	xx	x	x	xx	x	xxx	xxx	xx
Aug-16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sep-16	0	xxxx	xxx	xx	xx	xxx	xx	xx	x	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Oct-16	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	x	x	xx	x	xxx	xxx	xx	x	x	xx	x	xxx	xxx	xx
Nov-16	0	xxxx	xxx	xxx	xx	xx	x	x	0	0	xxxx	xx	xx	0	0	xx	0	xx	x	x	x	x	xx	x	xxx	xxx	xx
Dec-16	0	xxxx	xxx	xxx	xx	xxx	xx	xx	x	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Jan-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Feb-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Mar-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Apr-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
May-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Jun-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Sep-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Oct-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Nov-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx
Dec-17	0	xxxx	xxx	xx	xx	xxx	xxx	xx	xx	0	xxxx	xx	xx	0	0	0	0	0	0	0	x	x	xx	x	xxx	xxx	xx

Date	QUARTZ						ORE										FECR				UNTREATED SLAG									OFF-GAS			
	Fe	Si	Al	O	Ca	Mg	Fe	Cr	Si	P	S	C	Al	O	Ca	Mg	Fe	Cr	Si	C	Fe	Cr	Si	P	S	Al	O	Ca	Mg	C	O	H	N
Jan-15	x	xxxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Feb-15	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
Mar-15	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Apr-15	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
May-15	x	xxxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jun-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-15	x	xxx	xx	xxx	0	x	xxx	xxxx	xxx	0	x	0	xxx	xxxx	xx	xxx	xxxx	xxxx	xxx	xxx	xx	xxx	xxx	0	xx	xxx	xxx	xxx	xxx	xxx	xxx	xxx	xx
Sep-15	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Oct-15	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Nov-15	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Dec-15	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
Jan-16	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Feb-16	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Mar-16	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Apr-16	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	x	xx	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
May-16	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jun-16	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jul-16	x	xxx	x	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	x	xx	xxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xx
Aug-16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Sep-16	x	xxx	xx	xxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxx	x	xx	xxxx	xxxx	xxx	xxx	xxxx	xxxx	xxx	xxx
Oct-16	x	xxxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Nov-16	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Dec-16	x	xxxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jan-17	x	xxxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Feb-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Mar-17	x	xxxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Apr-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
May-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Jun-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Jul-17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Aug-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Sep-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Oct-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Nov-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx
Dec-17	x	xxx	xx	xxxx	x	x	xxxx	xxxx	xxx	x	x	0	xxxx	xxxx	xx	xxxx	xxxx	xxxx	xxx	xxx	xxx	xxx	xxxx	x	xx	xxxx	xxxx	xxx	xxxx	xxxx	xxxx	xxx	xxx

4.3.4 Visualising results

The data of the mass balance is visualised in various ways in order to see the results of certain key parameter indicators. The following visualisations will be provided:

- Cr from ore vs. Cr in FeCr product
- Fe from ore vs. Fe in FeCr product
- Total C in vs. C in product
- Total mass in vs. total mass out

Each of these visualisations will be provided and discussed briefly.

Cr from ore vs. Cr in FeCr product:

The amount of Cr in the ore, trended together with the amount of Cr present in the final metal product, ultimately gives an idea of the recovery of Cr from the furnace. This trend is shown in Figure 4-3.

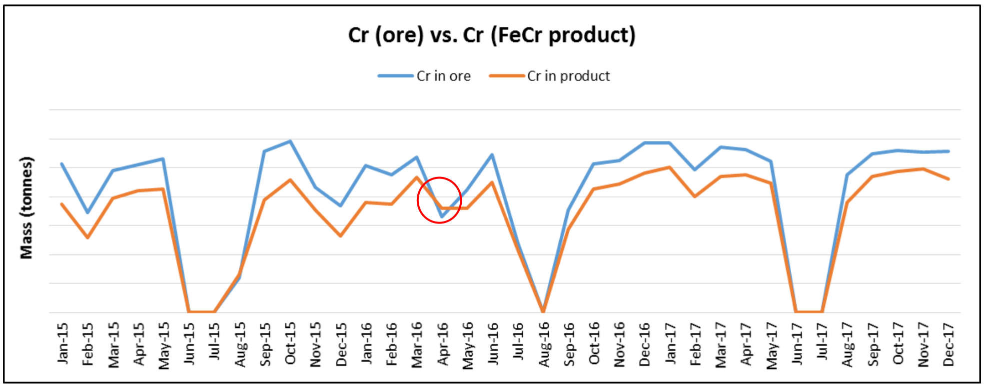


Figure 4-3: Cr from ore vs. Cr in FeCr product

These two lines must be as close together as possible, which would indicate that most of the Cr fed to the furnace is recovered in the final FeCr metal product. In this case, the relationship between the two streams seems to be typical, with the exception of April 2016. Here, the amount of Cr in the product exceeds the amount of Cr fed by the ore, which is not possible. Further data investigation can be done when such an incident occurs.

The variance between the two lines is calculated to be 18%, which means that there was a 100% - 18% = 82% recovery of chrome. This correlates well with the value found in literature (as stated in section 2.2: between 80 and 85%).

Fe from ore vs. Fe in FeCr product:

The visualisation of Fe is similar to that of the Cr, discussed in the previous point. The Fe trend is shown in Figure 4-4.

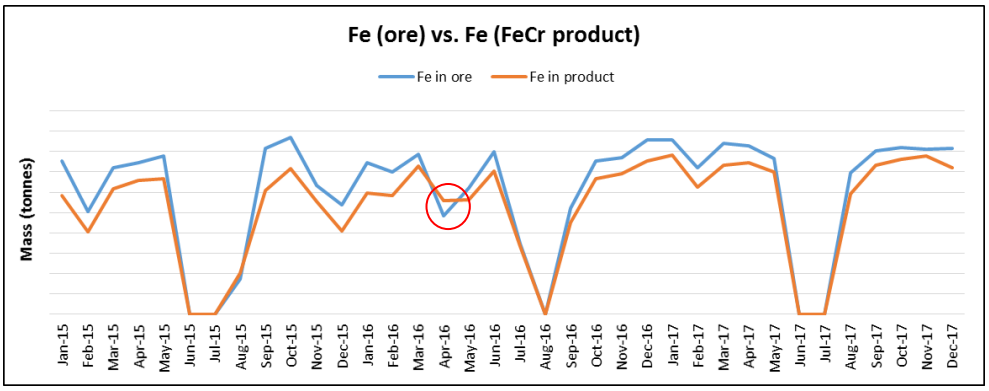


Figure 4-4: Fe from ore vs. Fe in FeCr product

Once again, the relationship between the two streams seems to be typical, with the exception of April 2016, as discussed previously. The difference between the variables is calculated to be 12%.

Total C in vs. C in product:

The total amount of carbon entering the furnace, trended together with the amount of carbon in the metal product, ultimately shows how much carbon is captured in the solid phase. The difference between the two lines would typically represent the amount of carbon emitted as part of the off-gas. The trend is shown in Figure 4-5.

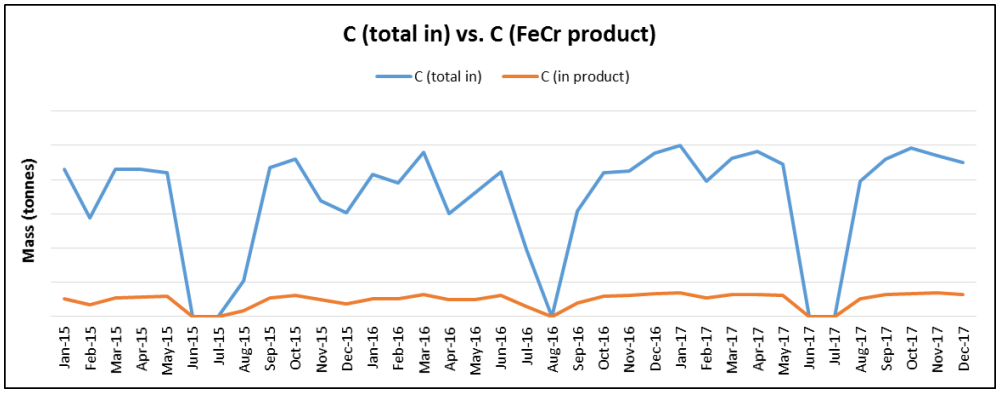


Figure 4-5: Total C in vs. C in product

It can be seen that the difference between the two lines is quite significant. The calculated difference is 86%, which means that 86% of the carbon used in FeCr production is emitted to the atmosphere (usually in the form of CO and CO_2). Further studies are in progress, focusing on off-gas emissions specifically [35].

Total mass in vs. total mass out:

The aim of this study is to perform a material balance on a typical ferrochrome furnace, which will be the final visualisation. The total mass of elements entering the furnace will be plotted against the total mass of elements exiting. This is shown in Figure 4-6.

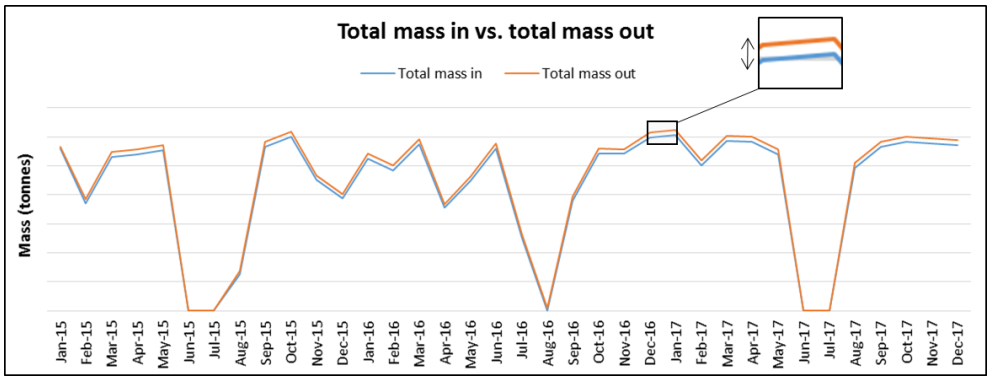


Figure 4-6: Total mass in vs. total mass out

Ideally, one would expect the two lines to follow the exact same trend, which would indicate a 'good' mass balance. This is almost the case, where a 1.25% discrepancy is found between the mass in and the mass out. This remains within the 3% error margin of an acceptable error, as chosen for this study.

Generally, the remaining results (not shown) also correlated well within the limits of typical mass ratios of input and output streams found in literature (as provided in section 2.2, p. 5).

5. CONCLUSION

This paper provided a brief overview of the furnace parameters measured in practice, before presenting an approach to perform the material balance. The available measurements of input and output streams were used together with compositions from literature. The analytical approach linked the known composition together with the known mass, to estimate the unknown streams.
The approach was applied to an industrial case study. The analysis managed to balance all elements (in and out) within an accuracy margin of 1.25%. Completing the mass balance up to this point can significantly decrease limitations on decision-making abilities.

6. BIBLIOGRAPHY

[1] **Gasik, M.M.** 2013. *Handbook of ferroalloys: Theory and technology*, Espoo: Elsevier.

[2] **Beukes, J., Dawson, N. & Van Zyl, P.** 2010. Theoretical and practical aspects of Cr(VI) in the South African ferrochrome industry, Infacon XII - Proceedings of 12th International Ferroalloys Congress, Helsinki.

[3] **Kühn, R., Geck, H.G., & Schwerdtfeger, K.** 2005. Continuous off-gas measurement and energy balance in electric arc steelmaking, *ISIJ International*, vol. 45, nr. 11, pp. 1587-1596.

[4] **Roos, J. & Hearn, A.** 2004. Optimising the effective use of energy in the ferroalloy industry through innovative technology, *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town.

[5] **Xiao, Y., Yang, Y. & Holappa, L.** 2006. Tracking chromium behaviour in submerged arc furnace for ferrochrome production, *2006 TMS Fall Extraction & Processing Meeting: Sohn Int'l Symposium*, pp. 583-594.

[6] **Otani, Y. & Ichikawa, K.** 1974. Manufacture and Use of Prereduced Chromium-ore, *Infacon I - Proceedings of 1st International Ferroalloys Congress*, Johannesburg,

[7] **Pan, X.** 2015. Effect of South African reductants on ferrochrome production, *Infacon XIV - Proceedings of Fourteenth International Ferroalloys Congress*, Kiev.

[8] **Pan, X.** 2015. Learning and teaching using process modelling and simulation, *International Conference on Mining, Minerals and Metallurgical Engineering*, Harare.

[9] **Ideas 1st Research.** 2010. *Ferrochrome*, Ideas 1st Research, Mumbai,.

[10] **Hattingh, J. & Friend, J.** 2003. Environmental and economic implications of slag disposal practices by the ferrochromium industry: A case study, *South African water research commission*, vol. 29.

[11] **Du Preez, S.** 2014. *Cr(VI) generation during flaring of off-gas from closed ferrochromium submerged arc furnaces*, North West University, Potchefstroom.

[12] **Basson, J., Curr T., & Gericke W.** 2006. *South Africa's ferroalloys industry - present status and future outlook*.

[13] **Sager, D., Grant, D., Stadle, R., & Schreiter, T.** 2010. Low cost ferroalloy extraction in DC-arc furnace at Middleburg Ferrochrome, *The Journal of The Southern African Institute of Mining and Metallurgy*, vol. 110, pp. 717-724.

[14] **Biermann, W., Cromarty, R. & Dawson, N.** 2012. Economic modelling of a ferrochrome furnace, *The Journal of The Southern African Institute of Mining and Metallurgy*, vol. 112, pp. 301-308.

[15] **Anon.** 2004. *Reductant characteisation in ferroalloys*, University of the Witwatersrand, Johannesburg.

[16] **Holappa, L.** 2010. Toward sustainability in ferroalloys, *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki.

[17] **Kapure, G., Kari, C., Rao, S.M.en Raju, K.S.** 2007. Use of chemical energy in submerged arc furnace to produce ferrochrome: prospects and limitations, *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi.

[18] **Riekkola-Vanhanen, M.** 1999. *Finnish expert report on best available techniques in ferrochromium production*, Finnish environment insitute, Helsinki.

[19] **Niemelä, P., Krogerus, H. & Oikarinen, P.** 2004. Formation, characteristics and utilisation of cogas formed in ferrochromium smelting, *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town,

[20] **Broekman, B. & Ford, K.** 2004. The development and application of a HCFeMn furnace simulation model for Assmang Ltd., *Infacon X - Proceedings of 10th International Ferroalloys Congress*, Cape Town.

[21] **Bergman, K. & Kjellberg, B.** 1997. *DC Arc Furnace Technology Applied to Smelting Applications*, Helsinki.

[22] **Harman, C. & Rama Rao, N.** 2007. Use of sintered pellets in production of high carbon ferrochrome, *Infacon XI - Proceedings of 11th International Ferroalloys Congress*, New Delhi.

[23] **Van Doorn, J., Bruyn, P. & Vermeij, P.** 1996. Combined combustion of biomass, municipal sewage sludge and coal in an atmospheric fluidized bed installation, *9th European bioenergy conference*.

[24] **Sun, Y., Sridhar, S., Seetharaman, S., Wang, H., Liu, L., Wang, X. & Zhang, Z.** 2016. A Fe-C-Ca big cycle in modern carbon-intensive industries: toward emission reduction and resource utilization, *Energy science and technology*.

[25] **Van der Sloot, H. & Cnubben, P.** 2000. *Verkennende evaluatie kwaliteitsbeinvloeding poederkoolvliegas*, ECN-report.

[26] **Klein, C. & Philpotts, A.** 2017. *Earth materials - Introduction to mineralogy and petrology*, Cambridge: Cambridge University Press.

[27] **O'Brien, M. & Wood, W.** 1998. *The prehistory of Missouri, Columbia*: University of Missouri Press.

[28] **Götze, J. & Möckel, R.** 2012. *Quartz: Deposits, mineralogy and analytics*, Heidelberg: Springer.

[29] **Hockaday, S.A.C. & Bisaka, K.** 2010. Some aspects of the production of ferrochrome alloys in pilot DC arc furnaces at Mintek, *Infacon XII - Proceedings of 12th International Ferroalloys Congress*, Helsinki.

[30] **Sprinzl, F.R.** 2016. *Valorization of ferrochrome slag: Towards increasing the beneficial utilisation of ferrochrome slag in South Africa*, Stellenbosch University, Stellenbosch.

[31] **Nkohla, M.A.** 2006. *Characterization of ferrochrome smelter slag and its implications in metal accounting*, Cape Peninsula University of Technology, Cape Town.

[32] **Herzog, T.N., Scheuren, F.J. & Winkler, W.E.** 2007. *Data quality and record linkage techniques*, Springer.

[33] **Booysen, W.** 2014. *Measurement and verification of industrial DSM projects*, North-West University, Potchefstroom.

[34] **Felder, R.M. & Rousseau, R.W.** 2005. *Elementary principles of chemical processes*, Hoboken (NJ): John Wiley & Sons, Inc.

[35] **Campbell, K.** 2018. *A critical analysis of emission quantification methods in the ferrochrome industry*, North-West University, Potchefstroom.

[i] Knowledge gained from site experience and interviews with site personnel
[ii] Knowledge gained from site experience and interviews with site personnel