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A MODEL FOR THE ANALYSIS AND THE PREDICTION OF EQUIVALENT CARBON DIOXIDE EMISSIONS IN THE PROCESS INDUSTRY

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Abstract

The aim of this thesis is to develop a mathematical model to analyze and predict the emission of greenhouse gases in the process industry.

The thesis project starts with the study of the EU ETS and the ISO 14064. These are the two main policies that provide guidelines to measure the impact of an installation in terms of greenhouse gas emissions.

Then, the overall scheme of the model is laid down, in compliance with both the EU ETS and the ISO 14064. The model relies on a matricial scheme and it is implemented with the software Matlab[®].

In order to validate the model, a case study on a specific industrial installation was performed. This case study consisted of tailoring the model on a existing facility and compare the outputs of the model with real data.

Finally, a techno-economic assessment evaluated the short and long term effects of process performances, energy price and carbon allowance availability on the balance of the installation subject of the case study. Additionally, a Montecarlo Simulation was performed to evaluate the economic risk that is linked to the future uncertainity of the EU carbon market.

Riassunto

Lo scopo di questa tesi è lo sviluppo di un modello matematico per analizzare e predire le emissioni di gas ad effetto serra di cicli produttivi industriali, su base oraria.

Il progetto di tesi è iniziato con lo studio del sistema di scambio di quote di emissione predisposto dall'Unione Europea (EU ETS) e con lo studio dello standard ISO 14064. ETS ed ISO 14064 sono le due normative più importanti che forniscono le linee guida per misurare l'impatto di una installazione in termini di emissione di gas ad effetto serra. Il sistema ETS impone un limite al volume totale dei gas ad effetto serra che vengono emessi dalle installazioni che devono aderire al sistema, e tale limite viene ridotto di anno in anno. L'adesione ad ETS è obbligatoria per le grandi installazioni energivore situate sul suolo Europeo, con l'aggiunta di Islanda, Liechtenstein e Norvegia. Tali installazioni aderenti devono rendicontare ogni anno le loro emissioni ed assicurarsi di pagare le quote di emissione corrispondenti. La ISO 14064, invece, è uno standard internazionale ad adesione volontaria che vuole apportare credibilità e garanzia ai processi di rendicontazione e monitoraggio dei gas ad effetto serra.

Successivamente, è stato ideato lo schema generale del modello, in conformità con le linee guida esposte nelle due normative appena citate. Il modello ha una struttura matriciale tridimensionale e viene implementato con il software di calcolo Matlab[®]. Il modello permette di ottenere una matrice contenente le emissioni orarie di una installazione, divise per categorie e per ora di interesse. Le categorie riflettono la struttura interna dell'installazione, in modo da permettere di discernere, ad esempio, l'attività che incide maggiormente sul volume totale di emissioni. L'ottenimento di questa matrice delle emissioni richiede una procedura ben precisa, divisa in step: il primo step è l'ottenimento dei dati per calibrare il modello sulle specifiche dell'installazione; il secondo step è l'elaborazione dei dati raccolti per disporli sulle matrici; il terzo, quarto e quinto step prevedono la generazione di matrici (tutte di uguali dimensioni) che contengono ognuna informazioni necessarie al calcolo delle emissioni, e la moltiplicazione tra di esse. Si ottiene così la matrice delle emissioni orarie.

Il modello è stato validato con un caso studio su una specifica installazione situata in Italia. Questo caso studio è consistito nel calibrare il modello su un impianto produttivo esistente, per poi comparare gli output del modello con i dati reali forniti dall'azienda che gestisce l'impianto. Il caso studio è servito non solo per costruire lo schema di monitoraggio e predizione delle emissioni dell'impianto, ma anche per verificare la bontà intrinseca della struttura del modello.

Infine, una analisi tecnico-economica ha permesso di valutare gli effetti a corto e a lungo termine delle prestazioni del processo, dei prezzi dell'energia e della disponibilità di quote di emissione sul bilancio dell'installazione soggetto del caso studio. In particolare, l'analisi ha coinvolto scenari della durata di 20 anni, e gli output analizzati sono stati il volume di emissione e l'incidenza dei costi di emissione sulla totalità dei costi di energia ed emissione, su base annua. Inoltre, è stata svolta una Simulazione di Montecarlo (MCS) per valutare il rischio economico connesso alla futura incertezza del mercato Europeo del Carbonio istituito con ETS. La simulazione ha valutato il rischio all'anno 2038 utilizzando gli stessi input ed output dell'analisi precedente.

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Introduction

Climate change has been identified as one of the greatest challenges facing nations, governments, businesses and citizens over future decades. Climate change has implications for both human and natural systems, and could lead to significant changes in resource use, production and economic activity. According to the last 2018 special report prepared by the Intergovernmental Panel on Climate Change, human induced warming reached 1°C above pre-industrial levels. In response, international, regional, national and local initiatives are being developed and implemented to limit greenhouse gas (GHG) concentrations in the Earth's atmosphere. As governments become aware of the scale of the problem, more and more measures are being taken to protect planet Earth and safeguard the well-being of its inhabitants. Such initiatives rely on the quantification, monitoring, reporting and verification of GHG emissions and/or removals. Putting a price on carbon is an extended measurement that many governments are taking to fight the enhanced greenhouse effect, which is the main cause of climate change, as agreed in the Kyoto Protocol. In addition, over the years, organization rights to emit will be cut down drastically in order to become a more climate neutral society. This is the background that gives birth to the necessity of driving technological development towards sustainable principles.

In this thesis, a model was created to address a necessity of this hystorical period. Indeed, establishing a detailed monitoring scheme, identifying the most impacting activities in terms of emission volumes to set up an improvement plan, predicting emissions to reduce performance losses, are just a few expamples of the many objectives that this model wants to achieve to ensure environmental sustainability in the industrial sector.

This thesis is developed as follows:

Chapter 1 presents the content of the EU ETS and the ISO 146064, which are the two main policies that provide guidelines to measure the impact of an installation in terms of greenhouse gas emissions.

Chapter 2 describes the overall mathematical scheme of the model and how it is used to describe the emissions of an industrial installation.

Chapter 3 is about the tailoring of the model on a existing installation through a case study. The installation is a glass factory located in San Giorgio di Nogaro (UD), Italy.

Chapter 4 deals with the possible future implications of the carbon market established by the European Union. A techno-economic assessment is performed to evaluate the influence of market prices and performance indicators on the budget of the glass factory.

Chapter 1

Initiatives on Climate Change: GHG inventories

After a brief presentation of the trends on GHG emissions in the last 30 years, this chapter introduces the two main approved policies that provide guidelines to measure the impact of an installation in terms of emission of greenhouse gases. The former was born with an European initiative to combat climate change and it is mandatory for heavy energy-using installations and airline operators. The latter is a voluntary-based European standard that is neutral with respect to GHG reduction programmes.

1.1 Global warming and the greenhouse effect

The greenhouse effect is a natural process which is indeed fundamental for the presence of life on Earth. Thanks to the presence of greenhouse gases (abbreviated as GHGs), part of the Sun radiation energy reflected by the ground is kept in the atmosphere, warming the surface of the planet. It has been estimated that without the greenhouse effect the average temperature of the planet would be -18 $^{\circ}$ C.

Since the industrial revolution, the intensification of human activities has been leading to a significant release of heat trapping gases known as GHGs. The build up of GHGs in the atmosphere enhances the greenhouse effect, altering the thermal equilibrium of planet Earth. As a consequence, human induced warming reached approximately 1°C (at least 0.85°C as a cautionary estimation) above pre-industrial levels as stated by the IPCC in their 2018 special report. According to the American Meteorological Society, of the 10 warmest years on record, eight occurred within the last decade. Of the two remaining, one occurred also in this century (2005) and one in the past century (1998). The warming of the planet also induced other life-threatening phenomena such as melting of the poles, rising sea levels, acidification of the oceans, extinction of species, massive migrations and extreme weather conditions, all of them ascribable to the climate change issue.

Table 1.1 lists all the types of greenhouse gases and the main activities that determine the emissions. The share of each greenhouse gas in the totality of emissions is determined by weighting each gas with a unique unit of measurement, i.e. tonnes of equivalent CO_2 . The equivalent CO_2 (CO_2e) is a unit for comparing the radiative forcing of a GHG with respect to carbon dioxide through the global warming potential. The global warming potential (GWP) compares the amount of heat trapped by a certain mass of a GHG to the amount of heat

Type of gas	Share in 2017	Source driver	Share in gas total in 2017
CO ₂	3%	Coal combustion	40%
		Oil combustion	31%
		Natural gas combustion	18%
		Cement clinker production	4%
		Subtotal drivers of CO ₂	92%
CH ₄	18%	Cattle stock	21%
		Natural gas production (incl. distribution)	13%
		Oil production (incl. gas venting)	13%
		Coal mining	11%
		Rice production	11%
		Landfill: municipal solid waste	8%
		Waste water	8%
		Subtotal drivers of CH ₄	83%
N ₂ O	6%	Cattle stock*	21%
		Synthetic fertilisers (N content)*	18%
		Indirect: atmospheric deposition, leaching and run-off (NH ₃)*	12%
		Crops	11%
		Fossil fuel combustion	11%
		Indirect: atmospheric deposition (NO _x)	7%
		Animal manure applied to solids*	4%
		Manure management	4%
		Subtotal drivers of N_2O , incl. relate drivers (*)	87%
F -gases	3%	HFC use	65%
		HFC-23 from HFC-22 production	19%
		SF6 use	14%
		PFC use and by-product	2%
		Subtotal drivers of F-gases	100%

Table 1.1. Key drivers of greenhouse gas emissions and global shares of main sources in2017. Source: EDGAR v4.3.2 and v5.0

trapped by a similar mass of carbon dioxide over a certain period of time, and is referred to carbon dioxide (whose GWP is standardized to 1). The Intergovernmental panel on climate change (IPCC) periodically publishes in their reporting guidelines a list of GWP reference values for a 100-year time horizon. For instance, nitrous oxide is 310 times more harmful than CO_2 while some fluorinated gas can reach values up to 23000. Please note that the GWP of methane has been re-evaluated over time. The second assessment report (SAR, 1996) of the IPCC indicated a GWP of 21 for methane while the fourth assessment report (AR4,



Figure 1.1. Global greenhouse gas emissions, per country and region expressed in Gt of CO₂e. Source: pbl.nl

2007) of the IPCC indicated a GWP of 24 (almost one-fifth larger). Officially, industrialised countries submit their annual national emissions inventory reports to the UNFCCC (United Nations Framework Convention for Climate Change) following the latest directions of the IPCC while developing countries follow the SAR. The 2012 revision of the ISO 14046 indicates the GWP directives from the SAR as well.

Since 1991, the European Commission has taken many climate-related initiatives to limit greenhouse gases emissions and to improve energy efficiency. With that being said, it is interesting to visualize the statistics of GHGs emissions from 1990 to the present day, with special interest on the role of the European Union in the global framework (see Figure 1.1). According to the 2018 report of the Netherlands Environmental Assessment Agency on the global GHGs trends, which relies on the most up-to-date databases provided by EDGAR (Emission Database for Global Atmospheric Research), the 28-group of the European Union is the third largest emitter of 2017 with a share of 9% of the total, preceded by the United States (13%) and China (27%), which has the primacy of largest emitter since 2004. In 2017 the growth in total global greenhouse gas (GHG) emissions has resumed at a rate of 1.3%per year, reaching a new greenhouse gas emission record of about 50.9 Gigatonnes of CO₂ equivalent (Gt CO₂e) (excluding those from land-use change) which is 55% higher than the emissions in 1990. Since the two previous years saw virtually no growth (0.2% in 2015 and 0.6% in 2016), there was a reason to think that global emissions could have eventually peaked. Unfortunately, the 2017 statistics ended this speculation. This rebound is mainly due to a new rise in global coal consumption (+0.7%), especially in India (+4.5%), twice the rate of 2016) and China (+0.2%), after three years of global declining coal consumption. This decline was caused by a decrease in coal consumption in China as well as declines



Figure 1.2. Global greenhouse gas emissions per type of gas and source, expressed in Gt of CO_2e . Source: pbl.nl

in the United States and the European Union, mainly from fuel switching to natural gas in power plants, and an increase of renewable power generation, in particular, wind and solar power. In contrast, global consumption of oil products and natural gas continued to increase, by 1.4% and 2.7% in 2017.

It is clear from Figure 1.2 that CO_2 is the most abundant greenhouse gas, so that its variation strongly influences the global emission trend. The dominant role of CO_2 arises from the fact that the main driver of CO_2 emission is the combustion of fossil fuels: more than three quarters of the total primary energy supply is fulfilled with combustion power (76%, 2017), the remaining with renewables (20%) and nuclear power (4%), as stated in the 2018 statistical review of world energy by British Petroleum.

Usually, total greenhouse gas emissions statistics do not include net emissions from land use, land-use change and forestry (LULUCF), which are accounted for separately. The LULUCF entry is inherently very uncertain and shows large interannual variations that reflects the periodically occurring strong El Niño years, such as in 1997–1998 and 2015–2016, as shown by the grey area above the dashed line in Figure 1.2.

In contrast with the global trend, GHG emissions of the EU are slowly, intermittently decreasing (see Figure 1.3). According to the 2019 inventory report of the European Environment Agency, total EU GHG emissions (excluding LULUCF) decreased by 1327 million



Figure 1.3. Histogram of EU-28 plus Iceland GHG emissions per year between 1990 and 2017, expressed in million tonnes of CO_2e . Source: eea.eu

tonnes since 1990 (or 23.5%) reaching their lowest level during this period in 2014 (4 307 Mt CO₂e). In the meantime, the GDP (gross domestic product) grew by 58%, proving a progressive decoupling between emissions and productivity. Few countries can claim the same successful result. For example, in the same period CO_2^{1} emissions grew by 354% in China and 305% in India because of their fast industrialization. The USA emissions remained almost unvaried (for both CO₂ and total GHG) while Russia decreased its GHG emissions by 32.4%. Almost all EU Member States reduced emissions compared to 1990 and thus contributed to the overall positive EU performance. UK and Germany accounted for about 50% of the total net reduction in the EU of the past 27 years, while the countries that increased their emissions are Spain, Cyprus, Austria, Ireland, Malta, Portugal and Iceland. In this period, Italy decreased its GHG emissions by 17.4%.

The reduction in greenhouse gas emissions over the 27-year period was due to a variety of factors, including the growing share in the use of renewables, the use of less carbon intensive fuels and improvements in energy efficiency, as well as to structural changes in the economy and the economic recession. Demand for energy to heat households has also been lower, as Europe on average has experienced milder winters since 1990, which has also helped reduce emissions. GHG emissions decreased in the majority of sectors, with the notable exception

¹Comparisons with China and India are carried out in terms of CO_2 emissions because the most recent data on GHG emissions date back to 2012 while CO_2 data are available until 2017. The comparison is still significant as CO_2 is always the most abundant GHG (between 70%-80%) in those countries.

of transport (including international transport), refrigeration and air conditioning. In addition to all the factors listed above, it is necessary to consider a number of policies (both EU and country-specific) that contributed to the overall GHG emission reduction, including key agricultural and environmental policies in the 1990s and climate and energy policies in the 2000s. So far, the most important EU policy of our century is the EU Emission Trading System (ETS), a plan introduced in 2005 to reduce GHG emissions by putting a price on carbon.

1.2 EU ETS: a mandatory legislative procedure

The EU emissions trading system (EU ETS) is one of the most important instruments of the EU's policy to combat climate change and reduce greenhouse gas emissions cost-effectively. The EU ETS is based on a cap and trade principle. It imposes a limit on the total volume of GHG emissions from installations and aircraft operators responsible of around 50% of EU GHG emissions. Within the cap, companies receive or trade emission allowances so that the total emissions of the installations and aircraft operators stays within the cap and companies are forced to take least-cost measures to reduce their emissions. Allowances are essentially rights to emit an amount of GHG equivalent to the global warming potential of 1 tonne of CO_2 equivalent (t CO_2e). The limit on the total number of allowances available ensures that they have a value. Furthermore, the size of the cap is decreased every year following a fixed scheme, ensuring the fulfilment of the long-term objectives of emission reductions.

There exist other national or sub-national carbon trading systems that operate or are under development in Canada, China, Japan, New Zealand, South Korea, Switzerland and the United States, but the EU ETS remains the biggest one, counting for over three-quarters of international carbon trading. Set up in 2005, it was the very first system of this type, operated in all EU countries (plus Iceland, Liechtenstein and Norway, which joined in 2008).

1.2.1 History and recent developments of the Cap and Trade System

The EU ETS is a policy instrument developed to meet the commitments of the 1997 Kyoto Protocol, which was agreed between 37 industrialised countries at the United Nations Framework Convention for Climate Change (UNFCCC). In order to meet the legally binding GHG reduction targets of the protocol, the European Commission presented some first ideas to start the foundation of ETS on a green paper dated March 2000. After several discussion with stakeholders, the GHG trading scheme was formalised into directive 2003/87/EC. The directive is dated 13th of October 2003, but the introduction of the system took place in 2005, engaging the first pilot phase.

The first period (2005-2007) was used to test price formation in the carbon market and to establish the necessary infrastructure for monitoring, reporting and verification of emissions. The main concern of this phase was to create the proper environment of learning-by-doing,

so that the new system could become a well-run procedure for companies and stakeholders. In addition, phase 1 gave the chance to update the caps with reliable data, since they were based on estimates.

Phase 2 (2008-2012) coincided with the first decrease in the availability of allowances i.e. the first emission cut on GHG, in agreement with the Kyoto Protocol.

The EU ETS is now in Phase 3 (2013-2020). A single EU-wide cap replaced the previous system of national caps. This EU-wide cap is designed to become increasingly stringent by a linear reduction factor of 1.74% per year. This allows companies to meet the increasingly ambitious overall target for emissions reductions.

The legislative framework for the upcoming Phase 4 (2021-2030) was revised in early 2018 in order to be in line with the 2030 climate and energy policy framework and as part of the EU's contribution to the 2015 Paris Agreement. The pace of annual reduction was speeded up by increasing the linear reduction factor of allowances to 2.2

From the start of phase 3 the system covers the following sectors and gases:

- Carbon dioxide (CO₂) from
- Nitrous oxide (N₂O)
- Perfluorocarbons (PFCs) from aluminium production.

In phase 1 the EU ETS covered CO₂ emissions. Voluntary inclusion of N_2O emissions was allowed from phase 2 at the discretion of EU Member States. Starting from phase 3 certain N_2O and PFC emissions were also covered. At the moment, the ETS does not cover methane emissions.

1.2.2 Achieving emissions reductions

The international community has agreed that global warming should be kept below a 2°C increase, as compared to the temperature in pre-industrial times. In 2008, the EU set a series of climate and energy targets to be met by 2020 in its pathway towards a low-carbon competitive economy, known as the "20-20-20" targets. These are:

- A reduction in EU greenhouse gas emissions of at least 20% below 1990 levels;
- 20% of EU energy consumption to come from renewable resources;
- A 20% reduction in primary energy use compared with projected levels, to be achieved by improving energy efficiency.

The targets were set by EU leaders in 2007 and enacted in legislation in 2009. In 2020, the target is for the emissions from the sectors covered by the ETS to be 21% lower than in 2005. In 2018 emissions from the sectors covered by ETS were reduced by 28% with respect to 2005 while total EU greenhouse gas emissions were reduced by 23% with respect



Figure 1.4. Total EU GHG emissions from 1990 to present days (solid blue) and future trends to be achieved in order to meet the anticipated 2020 (dashed blue) and 2030 targets (dashed red). Source: ec.europa.eu

to 1990. The new targets for 2030 are 40% cuts in total greenhouse gas emissions from 1990 levels and a 43% cut in emissions from the sectors covered by the ETS from 2005 levels (see figure 1.4).

By increasing the pace of allowance reductions, Europe is expected to drop its GHG emissions by 40% at the latest in 2030. The long term, most ambitious target will be achieving a climate neutral Europe by 2050. As the IPCC stated in 2018 in their special report, "limiting warming to 1.5° C implies reaching net zero CO₂ emissions globally around 2050 and concurrent deep reductions in emissions of non-CO₂ forcers, particularly methane".

In order to comply with the EU ETS, each year a company must surrender (i.e. return) enough allowances to cover all its emissions, otherwise heavy fines are imposed. A company can obtain allowances via free allocation or auctioning. From phase 3, the total amount of free allocation each installation should receive is determined by product-related GHG emission benchmarks, in this way installations that are highly efficient should receive all or almost all of the allowances they need to comply with EU ETS obligations. Inefficient installations have to make a greater effort to cover their emissions with allowances, either by reducing emissions or by purchasing more allowances. During phases 1 and 2, most allowances in all Member States were given out for free based on historical GHG emissions. On the other hand, auctioning is the default method of allocating allowances, meaning that all allowances not allocated free of charge will be auctioned. In 2013, over 40% of the allowances were auctioned, with this proportion continually rising throughout the trading period. Auctioning revenues have been used or are planned to be used for climate and



Figure 1.5. Principle of the EU ETS compliance cycle. Source: ec.europa.eu

energy purposes.

1.2.3 Compliance Cycle

Since the beginning of the third trading period in 2013, the monitoring and reporting of greenhouse gas emissions needs to be in line with the EU Monitoring and Reporting Regulation (MRR - Commission Regulation (EU) No 601/2012). The MRR creates an accurate and transparent compliance system that is essential for creating trust in emissions trading. When an installation enters the ETS, it has to submit a monitoring plan that must contain at least the information reported in Annex I of the MRR, including the description of the installation and its emission sources, the monitoring methodology and the responsibilities within the installation. This plan has to follow the principle of continuous improvement and has to be updated and re-approved whenever it is modified. In addition to that, every year operators of installations and aircraft operators need to hand in an Annual Emission Report (AER) that is in line with the MRR to the Competent Authority. The AER is the key document that provides the amount of emitted greenhouse gases of that operator in a given year.

The AER needs to be verified by an independent accredited verifier. The verification of emission reports and accreditation of verifiers need to be in line with the EU Accreditation and Verification regulation (Commission Regulation (EU) No 600/2012) from phase 3 as well. Both regulations (600/2012 and 601/2012) strive for a more harmonised MRV system in the EU. The principles of the EU ETS compliance cycle are graphically shown in Figure 1.5.

A tier system is adopted to define accuracy levels in which installations of different sizes need to report their emissions. The EU ETS classifies installations in three different monitoring categories (MRR, Article 19):

- Category A: average annual emissions equal to or less than $50,000 \text{ tCO}_2(e)$
- Category B: average annual emissions equal to or less than 500,000 tCO₂(e)
- Category C: average annual emissions higher than $500,000 \text{ tCO}_2(e)$

Installations are considered small emitters if they emit less than 25'000 tCO2e per year and, if they are combustion installations, have a thermal rated input below 35MW (MRR, Article 47).

As a general principle, operators of B and C installations are required to apply the highest tier (i.e. the most accurate) for each parameter. However, the operators may apply a tier one level lower than required for category C installations and up to two levels lower for category A and B installations, with a minimum of tier 1, in the case they show to the competent authority that the tier required is technically not feasible or incurs unreasonable costs (MRR, Article 26).

1.2.4 Monitoring approaches

The operator shall choose to apply one of the following methodologies:

- A calculation-based methodology, consisting in determining emissions from source streams based on activity data obtained by means of measurement systems and additional parameters from laboratory analyses or default values. The calculation methodologies should be further differentiated into a standard methodology (Article 24 of the MRR) and a mass balance methodology (MRR, Article 25). The standard methodology applies the following formulae for CO2 emissions, distinguishing between combustion and process emissions:
 - a) Combustion emissions

$$Em_c = EC \cdot EF \cdot OF \tag{1.1}$$

where Em_c are combustion emissions in tCO₂, *EC* is the energy content of the fuel in TJ, *EF* is the emission factor in tCO₂/TJ of fuel and *OF* is the oxidation factor which is dimensionless (it is used in case of incomplete reaction). The energy content is obtained with the following formula:

$$EC = FQ \cdot NCV \tag{1.2}$$

where FQ is the fuel quantity in tonne or Nm³ and NCV is the lower calorific

value in TJ per unit of fuel. Emission factors and calorific values are listed in Annex VI comma 1 of the MRR.

b) Process emssions

$$Em_p = AD \cdot EF \cdot CoF \tag{1.3}$$

where Em_p are process emissions in tCO₂, AD are activity data (i.e. the quantity of input material consumed or the resulting output of the process) in tonne or Nm³, EF is the emission factor in tCO₂/t of input/output material or tCO₂/Nm³ of input/output material and CoF is the conversion factor which is dimensionless (it is used in case of incomplete reaction). Emission factors are listed in Annex VI comma 2 of the MRR.

The mass balance methodology is especially useful when it is difficult to relate emissions directly to input materials because the products and wastes contain significant amount of carbon (e.g. bulk organic chemicals, carbon black). In these cases an oxidation factor or conversion factor is not enough to account for non-emitted carbon. Instead, a complete balance of carbon entering and leaving the selected installation boundaries is used. The mass balance on carbon is:

$$Em = \sum_{i} (f \cdot AD_i \cdot CC_i) \tag{1.4}$$

Where *i* is the index for the material or fuel under consideration, *f* is the factor for converting the molar mass of carbon to CO_2 , as specified in Article 25 of the MRR. Its value is 3.664 tCO₂/tC. *AD* is the activity data (i.e. mass in tonne) of the material or fuel, positive if they are entering, negative if exiting the process. *CC* is the carbon content of the compound under consideration, which is calculated as:

$$CC_i = \frac{EF_i \cdot NCV_i}{f} \tag{1.5}$$

where EF is the emission factor in tCO₂/TJ and NCV is the lower calorific value in TJ per unit of fuel.

It is important to underline that whenever biomass materials or fuels are included in the calculation, both the *EF* and *CC* have to be adjusted for the fossil fraction only because carbon contained in the biomass belongs to a closed cycle and has to be excluded from the calculation.

2) A measurement-based methodology consists in determining emissions from emission sources by means of continuous measurement of the concentration of the relevant greenhouse gas in the flue gas and of the flue gas flow (MRR, Article 40). The emissions are first determined per each hour of measurement from the hourly average con-

centration and the hourly average flowrate. Then, all hourly values are summed up for the total annual emissions of that emission point (MRR, Article 43). The continuous emission measurement system is defined as a set of operations having the objective of determining the value of a quantity by means of periodic measurements performed with an instrument that is inside or close to the stack. The collection of individual stacks is not allowed, which means that the measurement apparatus has to be fixed and countinuous operating.

- 3) An **alternative methodology**, also addressed as fall-back approach (MRR, Article 22), which can be proposed by the operator when the tier system is technically not feasible or leads to unreasonable costs. However, the operator has to demonstrate that the proposed alternative methodology allows to achieve the required overall uncertainty level for the emission of the total installation. In other words, instead of complying with the uncertainty of each source stream, one common uncertainty level for the total emissions of the installation is complied with. Since this approach requires much administrative effort (submission of yearly uncertainty assessments, demonstration of unreasonable costs or technical unfeasibility following the procedure in Article 18 of the MRR), it is advisable to use the other methodologies listed in this section.
- 4) A **combination of approaches** outlined above, on the condition that no data gaps and no double counting occur. In particular, the operator shall choose the methodology that allows to achieve more reliable results and the lower inherent risk of error.

When an installation fails to surrender (i.e. return) enough allowances, it has to pay an excess emission penalty of 100 euros per each tonne of CO_2e not covered (during phase 1 the penalty was 40 euros) (Article 16 of Directive 2003/87/EC).

1.3 UNI EN ISO 14046: a voluntary-based standard

The ISO 14064 is a three part international standard belonging to the ISO 14000 series of International Standard for environmental management. The ISO 14064 standard provides governments, businesses and other organisations with a transparent and reliable methodology to quantify, monitor, report and verify GHG emissions and/or removals.

The objective of ISO standards is to ease international cooperation, especially business and trade, by facilitating communication on technical issues between industry, government, consumers, and other stakeholders and allowing consistency of products and services within and across national boundaries. ISO 14064 exists as a guide for the private and public sector in developing GHG inventories for their organization. Even though the ISO 14064 standard is climate policy neutral, it facilitates the development and implementation of strategies and plans that address the global environmental challenge of climate change such as emission reduction or removal enhancements of GHG.

The text of ISO 14064 has been prepared by Technical Committee ISO/TC 207 "Enviromental Management" of the International Organization for Standardization (ISO). The development process included the involvement of over 175 experts representing 45 countries. The development of ISO 14064 began in 2002. Recognizing quickly emerging interest in addressing the environmental issue posed by climate change combined with the lack of international standards for businesses to take action, a work group was formed to fill the existing gaps between organizations and climate action. The norm was published in 2006 and reviewed in 2012 and 2018.

The standard is divided into three parts, each with a different technical focus. They can be used separately or altogether.

Part 1 is titled "Specification with guidance at the organization level for quantification and reporting of greenhouse gas emissions and removals". This part details principles and requirements for designing, developing, managing and reporting organization or company-level GHG inventories.

Part 2 is titled "Specification with guidance for the validation and verification of greenhouse gas assertions", and addresses quantification and reporting of emission reductions from project activities.

Part 3 is titled "Specification with guidance for the validation and verification of greenhouse gas assertions" and establishes a process for verification of a greenhouse gas statement, including organization inventories, regardless of whether or not the inventory was developed under Part 1. This verification process is also applicable whether the verification is being conducted by an independent third party verifier or by an organization's internal auditors. The requirements for GHG validation and validation bodies for use in accreditation or other forms of recognition are specified in the ISO 14065 standard.

1.3.1 Guidelines for inventory design

We now address the specific methodology of quantification of organization-level GHG, as described in the first part of ISO 14046.

ISO 14064, Part 1 includes eight major sections with over 21 subsections discussing GHG inventory issues for organizations. At the beginning, the standard establishes and defines general GHG inventory principles of relevance, completeness, consistency, accuracy, and transparency. These principles serve to assist with both interpretation of the standard as well as general guidance for addressing issues that fall beyond the practices established by the standard. The following section identifies three key aspects for developing a greenhouse gas inventory for organization. These aspects include setting inventory boundaries, quantifying GHGs, and reporting GHGs.

Boundaries for a GHG inventory include both the organizational boundaries and the operational boundaries.



Figure 1.6. Relationship between GHG sources, sinks and facilities inside the organizational boundaries. X is the number of facilities in the organization; n is the number of sources or sinks in a facility. Source: ISO 14064-1

Organizational boundaries (Figure 1.6) refer to defining which facilities are recognized as part of organization conducting the inventory and should be included within this inventory. The organization should choose between two approaches to defining organizational boundaries: by control or according to the equity share. Under the control approach, an organization looks at facilities where it has authority to implement either financial or operational policies, then accounts for all GHG emissions from facilities where it does have control. Under the equity share approach, the organization accounts for emissions from all facilities in which it has some equity interest (even a minority), but accounts for only a percentage of the total emissions equal to the share it has in the particular facility or sub-entity.

Operational boundaries refer to which operational activities at a facility are included in the inventory. Once they are identified, they need to be categorized into direct emissions, energy indirect emissions and indirect emissions. Direct GHG emissions, or emissions that result from activities directly under an organizations control, such as combustion of fossil fuels to generate heat, are always included within the inventory. Indirect GHG emissions, or emissions that result from organization activities but are generated outside the boundaries of the organization's direct control, may or may not be included. Indirect emissions from electricity generation are always included but other indirect emissions, such as those resulting from employee travel in non-organization owned vehicles (e.g. commercial airlines) are optionally included.

After setting the boundaries, the standard identifies five steps for quantification of GHGs.

The first two steps of this process are identification of specific emission sources within the operational boundaries as well as selection of an emissions quantification methodology applicable for the sources identified. The next steps are the collection of data required by the methodology for the source and the identification of established emission factors for the data collected. Finally, the data and the emission factors, applied consistent with the quantification methodology, are used to quantify emissions from individual emission sources. The emissions quantified for each source are then consolidated with the other sources within the operational boundaries, but ensuring that direct and indirect sources are kept separate.

With respect to GHG inventory reporting, ISO 14064 establishes that the report for each reporting period should identify the entity's organizational boundaries, the GHG emissions from individual operational categories, and the methodologies used to quantify those emissions. The report should include appropriate explanation regarding these inventory components, especially any modification introduced to the methodology or the organization boundaries, with its explanation. The report should also identify what particular standards (including ISO 14064 for example) or programs the inventory was conducted consistent with and whether verification relative to these standards or programs was undertaken.

1.4 Comparison between the two inventory procedures

The previous sections (§1.2 and §1.3) described how the inventory of greenhouse gases is performed according with the two main policies on the matter. Now, the charachteristics of the two policies are compared.

The first and most important aspect to be kept in mind is the different condition of accession to the two procedures, even though the purpose remains mutual. In fact, the EU ETS is a legally binding European directive addressed to all member states. This means that all member states must transpose and implement it correctly. The ISO 14064, instead, is an international standard addressed to any world country that can be adopted solely on a voluntary base.

The second aspect is the fact that the EU ETS only addresses industrial plants that emit via combustion or process emissions. For this reason, methane is not included in the inventory and the reporting of N_2O and F-gases is mandatory only for a restricted group of industries (nitric, adipic and glyoxylic acid production for N_2O and aluminium production for F-gases). On the other hand the ISO 14064 requires organizations to account for all the four types of GHG and is addressed to all kinds of organizations, either public or private.

The third aspect is the fact that the ISO 14064 accounts for certain types of emissions, categorized as indirect emissions, that are not taken into consideration into the EU ETS. We are talking about energy indirect GHG emissions which are generated from imported electricity, heat or steam used by the organization, and other various indirect emissions, at

the discretion of the organization boundaries selection, such as commuting and business travel by employees or transportation of organization's products, material, people or waste by another organization.

1.5 Study objectives

As seen above, putting a price on carbon is an extended measurement that many governments are taking to combat the enhanced greenhouse effect, which is the main cause of climate change as agreed in the Kyoto Protocol. In addition, over the years organization rights to emit will be cut down drastically in order to become a more climate neutral society. This is the background that gives birth to the necessity of driving technological development towards sustainable principles.

The objective of this study is to create a model that is able to proactively monitor and predict GHG emissions of an industrial installation in a systematic way, with the aid of a computational software. This model is structured as an inventory that performs the accurate counting of all the equivalent carbon dioxide produced by an installation. Emissions will be estimated on a hourly basis, correlating environmental performances with expected production profiles through the knowledge of empirical data on the production site. The forecasting of emissions allows to monitor potential performance losses of the installations by comparing expected profiles with real data provided by sensors. Deviations from ordinary marching operations can be spotted right away, and they can be quantified in terms of carbon allowances. Moreover, the model allows speculating on potential short and long term scenarios, accounting for the variability of process indicators, energy price and carbon allowances.

In order to validate the model, a case study on a specific industrial installation will be proposed. So, the original model is specifically tailored to the scheme of a glass factory located in San Giorgio di Nogaro (Italy) that produces flat and laminated glass using state-of-theart technology. Eventually, an economic risk assessment is carried out with a Monte Carlo Simulation to consider the impact of energy efficiency and costs generated by the emission of greenhouse gases.

1.6 State of the art of available models

A number of models that pursue the same environmental aim are found in the literature. Some examples from different sectors are collected in this section.

Drawing attention to the heavy industry sector, which accounts for a large share of global anthropogenic gases, Ruijven *et al.* (2016) simulated a comprehensive scenario for the steel and cement industry developing projections of energy use and CO_2 emissions at different levels of carbon taxes. Following this route, Sen et al. (2016) forecasted energy and GHG emissions for an Indian pig iron manufacturing to achieve better environmental management

practice.

The construction industry is a major contributor to global GHG emissions as well, and it is directly related to urbanization. On this matter, Liu *et al.* (2019) developed a real-time monitoring of greenhouse gas emissions in construction sites. Data are collected on site and transmitted to a remote server. Subsequently GHG emissions are displayed using a quantitative model. Regarding the single building, Brännlund and Nordström (2004) modelled a household demand located in Norway, analysing consumer response due to changes in energy or environmental policy (in particular, a doubling of the carbon tax is considered).

Another relevant sector is transport: Kamiya *et al.* (2019) modelled the GHG emission intensity of plug-in electric vehicles with a well-to-wheel analysis, depending on the sustainability of the electricity source.

In the agricultural sector, Gocht *et al.* (2016) modelled the dynamics of carbon fluxes as it is sequestrated from the atmosphere thanks to a grassland increase of 5% in the EU. The substantial cost of carbon sequestration per ton CO_2 was calculated as well.

Finally, Zaroni *et al.* (2019) used a Monte Carlo Simulation to assess the economic risk of investment on an emergency generator system for a Brazilian campus. The study considers different rated powers of diesel and natural gas-based generators as well as emission costs linked to carbon credits.

Chapter 2

Development of a model to predict CO₂e emissions

This chapter explains how the model was developed and all its characteristic features. After a brief introduction on the genesis of the model and its purposes, a detailed step-by-step procedure is provided to explain how the model was built. Finally, the outcomes of the model are presented and the benefits of adopting this model as an action towards more sustainable principles are discussed.

2.1 Introduction to the model

The model is intended as a compact scheme to analyse and predict CO_2 emissions from an industrial installation. The importance of creating this model lays in the necessity of proactively monitoring greenhouse gases emissions, as they are the main cause of climate change. As seen in the previous chapter, keeping track of emissions is the starting point for environmental action in the industrial sector. By facilitating the accounting of emissions, this model helps identifying the most critical areas of the specific installation where it is advisable to improve energy or process efficiency.

The idea to develop this model came from Ing. Luca Vecchiato, an expert of energy management who has been working in the sector of energy consulting for 20 years. Back in the days Ing. Vecchiato developed his own energy model that has proven to be successful over the years. The energy model has been used for energy audits (i.e. analysis of the energy consumed by an installation with the purpose of increasing energy efficiency, as laid down in Legislative Decree No 102 of July 4th 2014) and for the certification of energy-related standards. The energy model developed by Ing. Vecchiato is the starting point for the development of the new CO₂e model proposed in this thesis. The old model accounts exlusively for energy flows and is based on a yearly balance, while the new model is designed to account for all the fluxes that generate equivalent carbon dioxide emissions, and it scales the time detail down to the hourly basis. The two models are similar, beacuse they rely on the same matricial scheme as detailed later. However, the introduction of a time-wise description in the new model requires the addition of a variable in the scheme, i.e. the addition of the third dimension in the matrix.

For completness, the CO₂e model was developed with the intention of complying with both of the policies illustrated in the previous chapter.

The CO₂e model is a procedure that results a tridimensional matrix containing data on hourly emissions, here referred to as CO_2e map. The most important step of the development of this model consists of sorting a large number of data in a meaningful way and perform several mathematical operations between data in a systematic manner. Therefore, the matrix seemed the most suitable and versatile mathematical scheme for this application. It should be mentioned that in the context of this thesis the words map and matrix have the same meaning, therefore they will be used interchangeably. The whole model was implemented with the use of the calculation software MATLAB[®].

2.2 Model structure

In order to organize the available information, the CO₂e model sorts data by categories of use and categories of consumption, on a hourly basis. These categories are described later in the paragraph. The core of the model are tridimensional matrices, which are made up of rows, columns and pages, as specified in Figure 2.1. Categories of use are represented in the columns, categories of consumption are represented in the rows and time is distributed along pages. It means that, for instance, in the CO₂e map each column describes emissions of a single category of use, each row describes emissions of a single category of consumption and each page describes emissions on a specific hour. An example of category of use that is usually present in all the installation is the internal lightning, powered by electricity, and the heating of the building, usually by gas or electricity, followed by other specific activities that are carried out in the plant, each one of them powered by an energy vector. An example of category of consumption is the operating hours of a specific production line or the throughput of a specific product. Categories of use and categories of consumption are designed to allow the breakdown and the sorting of data into groups. Each element of the matrix describes the equivalent carbon dioxide emissions for a specific use and a specific consumption in a given hour, determined by the position of the element in the matrix. Once categories are distributed, their positions remain unvaried for all the matrices (i.e. all the maps).

Categories of use describe emissions based on the purpose of the process that generated them. Moreover, each category of use relies on a single energy vector, which could be a primary or a secondary energy vector. *Primary energy vectors* are those entering the boundaries of the installation and utilized "as-is". *Secondary energy vectors* are those obtained by transformation of the primary vectors inside the boundaries of the installation. Categories of consumption sort emissions depending on the throughput of a product or hours of operation of a process. These categories are identified based on the specific installation. For better understanding, a brief example is provided.

A factory produces product A and product B. The same factory employs the following equipment: a gas boiler to heat up the raw materials in production line A, an electrical conveyor


Figure 2.1. Scheme of a multidimensional array with three dimensions: each element is defined by three subscripts, the row index *x*, the column index *y* and the page index *z*. The first two dimensions are commonly represented in classical 2D matrices, but the third dimension represents pages or sheets of elements.

belt to move the raw materials in production line B and a LED lightning system connected to the electrical system. Hypothetically, the following categories of use could be identified: process heating with gas, moving machinery by electricity and internal lightning by electricity. In the same way, the categories of consumption could be: throughput of product A, troughput of product B, hours of operation of production line A and hours of operations of production line B. To complete the model one should collect a number of data such as the time schedule of production lines and their productivity, the rated power of equipment and the specific energy consumption of each piece of equipment. The information required to build the model are described in the next section.

2.3 Model development

The CO_2e model relies on a calculation-based methodology. The principles of a calulationbased methodology are described in paragraph §1.2.4. This methodology consists of determining CO_2e emissions by multiplying the energy content of a vector or the activity data of a process input with a series of conversion factors (Figure 2.2). Since an industrial installation can potentially use many energy vectors and process inputs, the number of operations to be performed may bevery large. The CO_2e model handles this problem by storing the relevant data into large matrices and by grouping together all the thousands of single operations into a unique (element-wise or scalar) multiplication between matrices.

Accordingly, the CO₂e model calculates emissions from energy vectors as follows:



Figure 2.2. Principle of the calculation-based methodology for calculating CO2e emissions of an installation. Emissions are calculated starting from input activity data on process materials and energy vectors which are multiplied by emission factors and further factors.

$$Em_c = SP \cdot SCH \cdot CF \cdot NCV \cdot EF \tag{2.1}$$

where *SP* is the specific consumption of an energy vector per hour or per tonne of product, *SCH* is the scheduled time production (on/off setting depending on wheter the process is working) or scheduled productivity (quantity of product produced per hour), *CF* is a conversion factor that converts from secondary to primary energy vectors (if necessary), *NCV* is the lower calorific value (applies only to fuels) and *EF* is the emission factor of the energy vector (ton CO_2 per unit of energy vector consumed). For completeness, energy indirect emissions from the generation of imported electricity, heat or steam are accounted in the model as well. For instance, when calculating electricity emissions, the calculation simplifies to *SP* (specific consumption of energy per hour or per tonne of product) times *EF* (electricity emission factor in ton CO_2 per kWh).

The CO₂e model calculates process emissions as follows:

$$Em_p = AD_s \cdot SCH \cdot EF \tag{2.2}$$

where AD_s is the specific activity data of an input material per hour or per tonne of product, SCH is the scheduled time production (on/off setting depending on wheter the process is working, implemented as a 1/0 switch) or scheduled productivity (quantity of product per hour) and EF is the emission factor of the material (ton CO₂ per unit of material).

The information on the hand right side of Equations 2.1 and 2.2 are stored in matrices. The



Figure 2.3. Block diagram that summarizes the procedure adopted to build the CO₂e model. The procedure is divided in four steps addressed in roman numbers (I, II, III, IV, V). Consecutive steps are delimited by an horizontal dashed line. Matrices are indicated within boxes.

result of the calculation, i.e. the left side of Equations 2.1 and 2.2, is a matrix too, as it results from a multiplication between matrices, and it is named " CO_2e map". The whole process outlined above is summarized in Figure 2.1 and can be broken down in five steps (I, II, III, IV, V). The procedure is implemented with the help of the software MATLAB[®].

The first step (I) is the collection of a large number of data about the installation under investigation. Once the boundaries of the installation are established, it is necessary to identify all the sources and sinks of GHG associated with the installation operations. Then, information on all the activities that determine process emissions, combustion emissions and energy indirect emissions are needed. Data required in step I may be found by doing a survey at the installation of interest. This is done by direct interaction with the employees and an on-site investigation.

The second step (II) is data processing. This means sorting data into categories of consumption and categories of use. For each combination of category of use and category of consumption it is necessary to identify the respective time schedule, production schedule and specific energy consumption. Once the categories are set, they are distributed along rows and columns, and this disposition remains unvaried for all the maps along all the steps. Consequently, from step II onward all the maps have the same dimension, which is the number of categories of consumption times the number of categories of use times 8760. The size of the third dimension (8760 pages) is the number of hours in a year, which is the pursued time detail. It is preferable to order categories of use based on the energy vector so that categories that rely on the same energy vector are next to each other.

The third step (III) includes the generation of the base map, the generation of the profiles map and the generation of the conversion map no. 1.

The base map contains the specific consumption (*SP*) of energy and the specific activity data (AD_s) of process inputs of each category identified before. Elements are arranged in order to match with the corresponding category on the map. The base map has 8760 pages that are identical only if specific consumptions are constant along the year.

The profiles map contains information on time schedule and production schedule (SCH) of each category. Schedules are defined as 1x1x8760 vectors that are arranged in order to match with the corresponding combination of categories on the map. A time schedule is a sequence of zeros and ones that describes wheter the process is running or not in the corresponding hour. Zero means off and one means on. In a standard industrial installation there could exist a large number of time schedules. For instance, the air conditioners for summer cooling have a different time schedule than the winter heating. Product A, that is produced for 8 hours a day, has a different time schedule than product B, that is produced for 18 hours a day.

A production schedule, instead, describes how much product is produced or is planned to be produced hourly (unit of product per hour).

The conversion map no. 1 contains information on the conversion factors (CF) needed to convert energy consumptions from secondary energy vectors to primary energy vectors. Elements are arranged in order to match with the corresponding category on the map.

The fourth step (IV) includes the multiplication between the base map, the profiles map and the conversion map no. 1 to obtain the primary map. Step four also includes the generation of the conversion map no. 2. The conversion map no. 2 contains information on the conversion factors (*NCV*, *EF*) needed to convert energy consumptions from primary energy vectors to ton of CO_2 and to convert the amount of process input materials to ton of CO_2 .

The fifth step (V) includes the multiplication between the primary map and the conversion map no. 2 to finally obtain the CO_2e map.

2.3.1 Conversion and emission factors

Conversion factors (*CF*) are used to convert secondary energy vectors to primary energy vectors. This conversion is required as it would be impossible to determine the volume of emissions of, for example, one normal cubic meter of compressed air. Therefore, first it is determined how much electrical energy is required to generate one normal cubic meter of compressed air through a conversion factor, and then an emission factor for electricity can be applied. The conversion factor from secondary to primary energy vectors inherently depends on the charachteristics of the machinery used to performed the conversion. For example, the conversion from the thermal power of an inverter air conditioner (secondary energy vector) to electricity (i.e. the primary energy vector from which it powers) requires the knowledge of the coefficient of performance (COP) of the chiller unit and the energy efficiency ratio (EER) of the heating unit.

By definition, an emission factor (*EF*) is the average emission rate of a greenhouse gas (in ton CO2e) relative to the activity data of a process input or a primary energy vector, assuming complete oxidation for combustions or complete oxidation for all the other chemical reactions. Emission factors are used to convert primary energy vectors and activity data of process inputs into the corresponding volume of CO₂e released. For combustion emissions, the emission factor is expressed in relation to the energy content (*NCV*) of the fuel rather than its mass or volume. Both the *EF* and the *NCV* are values of paramount importance for the exact calculation of emissions. Both the ETS and the ISO 14064 have a dedicated literature that references the IPCC 2006 Guidelines for the values of *EF* and *NCV*. Alternatively, when a higher level of accuracy is required by the policy, the emission factor and the net calorific value may be specifically determined by requesting chemical analyses to external certified laboratories.

2.4 Model Outputs

When correctly applied, this CO_2e model allows to obtain a series of important information on the hourly variation of GHG emissions along the year. Moreover, it is possible to extract information on the variation of energy and process input consumptions along the year. Thanks to the matricial scheme introduced into the model, it is possible to recognize which category determined the largest volume of emissions or which category is the most energy-intensive.

The information extracted from the analysis of the model outputs are useful to set up a plan to identify opportunities of improvements. In a perspective of continuous improvement, these opportunities are aimed to improve resources usage and decrease the volume of emissions, observing the concept of the Deming cycle (Plan-Do-Check-Act).

In addition, the comparison between the model results and real time data (if available) is a

potential way to determine wheter the process drifts from the normal opertaing conditions. For better understanding this model capability, an example is provided. An installation is expected to produce 10 tons of product A per hour with a specific energy consumption of 30 kWh per ton. Product A is produced on production line A, which is powered with a dedicated eletrical supply cabling. The supply cabling of line A is equipped with a current transmitter that sends to a data logger the information on how much energy flows through the cable. The CO_2e model, calibrated on this specific installation, predicts that in the next hour 300 kWh will be consumed, as expected. This prediction is compared with the real data on electricity consumption that comes from line A. The real data is 500 kWh, measured in the same hour as the predicted value. Now, within an appropriate tolerance between the predicted and the real data, one could state with confidence that a malfunction exists. This malfunction is spotted right away, without waiting for the day to end or even for the next bill to arrive. Moreover, saving energy and materials means generating less emissions, greener production and less carbon allowances to be purchased.

Chapter 3

Case study on a industrial installation

This chapter shows how the model developed can be applied to analyse the emissions of an existing industrial installation through a case study. After a detailed description of the installation, this chapter illustrates step by step the process that allowed to tailor the model to the specific installation under consideration. Finally, the results of the calculations are analyzed and discussed.

3.1 The glass factory

The installation subject of this case study is a glass factory located in San Giorgio di Nogaro (UD) in the north-east of Italy. This plant is continuously operated and produces flat glass and laminated glass. With an average productivity of 600 tons of flat glass per day and more than 200 thousand tons per year, this factory is the largest producer of flat glass in Italy. In addition, since 2016 the plant has been owned by the Turkish group Sisecam which is the largest producer of flat glass in Europe, positioned among the top three worldwide.

3.1.1 Production process

The modern technology to produce flat glass was invented by Pillinkton in 1959 and is called float glass process. In the float process a continuous ribbon of glass moves out of a melting furnace and floats along the surface of an enclosed bath of molten tin (Figure 3.2). Here follows a detailed description of the float glass process and the operations that are carried out in the plant.

The production of flat glass starts from the collection of raw materials, principally sand, soda, limestone and dolomite, which are kept in different silos. After being weighed separately they are mixed and then poured into the charging hopper along with the glass cullet (crushed scrap glass). All these operations are fully automated and they take place in a section of the plant which is called *batch house*. Several batches of raw materials are fed to the oven every day.

The raw materials are melted in the furnace at a temperature of 1550°C produced by powerful gas burners. As it melts, the mixture vitrifies and flows slowly down inside the furnace, undergoing a process known as "fining". During this operation, the molten glass is kept at a high temperature for several hours, enabling bubbles of carbon dioxide to free themselves out from the carbonates.



Figure 3.1. Block Flow Diagram of the production pocess of flat glas, from the mixing of raw materials (top left) to the shipping of the finished product (bottom left).



Figure 3.2. Scheme of the production pocess of flat glass, from the mixing of raw materials (left) to the cutting of the chilled glass strips (right).

As it comes out of the furnace, the molten glass is poured onto a bath of liquid tin, where a sheet of glass called "ribbon" is formed by flotation. The tin bath and the ribbon are held in a chemically controlled atmosphere of 10% H₂ and 90% N₂. From one end of the bath to the other one, the temperature of the glass and of the tin gradually drops from 1100° C to 600° C. At this lower temperature the glass is hard enough that the rollers do not leave trace on the lower surface. A steady state thickness is achieved on the molten tin. The manufacture of thinner or thicker glass is possible with the help of top rollers. These are toothed wheels that lie on the edges of the ribbon and they draw out the glass mechanically to give it the required thickness and width depending on the angle of the force they exert.

The continuous strip of glass is moved by a roller conveyor from the end of the tin to an

annealing tunnel, known as *lehr*. Here, the glass is gradually reheated with resistances and cooled with fans in a controlled way, in order to ensure perfect flatness and eliminate any internal mechanical stresses which could cause breakage. The glass comes out of the *lehr* at ambient temperature, ready for cutting.

After annealing, the glass strip is inspected by an optical laser system to spot defects, and then automatically cut into large sheets. The edges are always cut off because they contain inhomogeneities. These sheets are sorted into orders and they are laid on stillages by automatic stacking machines, ready for shipping. In addition, these sheets are used in the plant to produce laminated glass, which is made up by an assembly of two or more sheets of glass with one or more plastic separation layers made of PVB (polyvinylbutyral). Depending on its composition, the laminated glass ensures greater protection for property (against break-in) or for people (against gunshot, explosion or risk of falling through).

In order to enhance the performances of the bare sheet, other additional treatments exist, such as thermal and chemical toughening, layers assembly and coating via deposition.

3.2 Model application to the specific installation

In order to apply the model to the glass factory it was necessary to know all the details and the characteristics of the installation. Hence, the first part of the case study focused on this task. Information regarding energy consumption, productivity and how energy and materials flow through the plant, eventually determining greenhouse gases emissions, were collected. This installation is of particular interest because it involves process emissions (CO_2 released from carbonates), combustion emissions (CO_2 released by the combustion of fuels) and also indirect energy emissions from the generation of imported electricity. This analysis was aimed to model the emissions of the installation in 2018.

3.2.1 Data collection and processing

The technical office of the company provided the precise information about the productivity and the energy consumption, including the amount of flat glass produced daily, the amount of gas consumed daily and the amount of electricity consumed daily.

An inventory of all the energy-consuming devices that are present inside the boundaries of the site was made. It was necessary to identify the characteristics of each device in terms of timing and extention of energy or process inputs consumption. For instance, electrical devices were characterized in terms of rated power, load factor and hours of use; gas burners were characterized in terms of gas combusted per ton of melted glass pulled from the oven, and so on. The amount of carbonates consumed as raw materials was related to the amount of glass pulled out of the oven by dividing the amount of carbonate consumed each month by the amount of flat glass produced in the same month. All the devices identified can run either on a primary or a secondary energy vector. Regarding the specific installation, the glass factory uses gas, electricity and diesel as primary energy vectors, although diesel is used only for emergency generators. Concerning secondary energy vectors, they are steam, compressed air and diathermic oil.

Following the general scheme described in the previous chapter, the model relies on 3-by-3 matrices, often referred to as *maps*. In order to build the rows and the columns of the matrices the devices were sensibly divided into 22 categories of use. Similarly, 5 categories of consumption were identified. The categories of use represent the columns of the model, while the categories of consumption represent the model rows. All the categories are listed and described in the next paragraphs.

The categories of use that were identified in the glass factory are listed below. For each category the primary energy vector from which it depends is indicated in brackets (except for carbonates, which are not generated by any vector). The unit of measurement of electricity is kWh. Gas is a mixture containing mostly methane. The categories of use are:

- 1-3) Carbonates, used as raw materials and mixed to the other ingredients in the batch house before being poured into the oven. Carbonates decompose under heating and release carbon dioxide. Three types of carbonates are used: sodium carbonate, calcium carbonate and dolomite. Each one has its own column and is measured in tons;
 - 4) Combustion heat (gas) provided by burners positioned on the sides of the oven. As soon as the gas enters the oven it ignites instantaneously creating an open flame that lays on top of the vitreous mixture. The gas flow is inverted every 20 minutes, so that the burners work alternatively. Natural gas is measured in standard cubic meters;
 - 5) Steam (gas) produced by a gas boiler and used to heat and humidify the raw materials mixture. Steam energy is measured in kWh of thermal energy;
 - 6) Diathermic oil (gas) heated in a gas boiler and used to assembly laminate. Oil energy is measured in kWh of thermal energy;
 - 7) Heating of the raw material mixture by means of an electrical boiler (electricity);
 - 8) Heating processes (electricity): heating in the annealing tunnel thanks to resistances placed over the glass ribbon and adhesion-heating of PVB for the laminate;
 - 9) Blowers for combustion air (electricity). The air is driven in a refractory tunnel where it is pre-heated with the residual heat recovered from the flue gases, and then it is directed to the oven.
- 10) Cooling processes (electricity): fans in the oven section, over the bath tin and in the annealing section; chillers to preserve PVB, chillers for air handling unit and others;

- 11) Moving machinery and other large equipments (electricity): conveyor belts and mixers for raw materials, top rollers to drag and move the glass ribbon, scanners, crane cutters; autoclave, air compressors and dryers for laminate;
- 12) Forklifts and cranes in the warehouse (electricity);
- 13) Compressed air (electricity) used for pneumatic conveyors to move raw materials. It is measured in normal cubic meters;
- 14) Off-gas handling (electricity): monitoring, electrostatic precipitation and pressurization;
- 15) Air cooling circuit (electricity). The water that flows in the water coolers inserted through the side walls of the forming section (tin batch) is cooled with air. This air is driven by air coolers ventilators.
- 16) Central water supply (electricity): pumps to extract water from the well and pressurize it in the circuit, water reintegration.
- 17) Diesel for emergency generators;
- 18) Wintern heating of the building with 46 inverters air conditioners (electricity);
- 19) Summer cooling of the building with 46 inverters air conditioners (electricity);
- 20) Internal lightning with more than 2000 bulbs and tubes (electricity);
- 21) External lightning of the forecourt with 86 bulbs (electricity);
- 22) Small electrical devices such as computers, printers and servers in the data processing center (electricity).

The categories of consumption that were identified in the glass factory are:

- 1) Specific consumption per tonne of flat glass pulled out of the oven;
- 2) Specific consumption per tonne of laminated glass produced;
- 3) Specific consumption per hour of production of flat glass;
- 4) Specific consumption per hour of production of laminated glass;
- 5) Other specific consumptions per hour.

3.2.2 Matrices calculations

The procedure followed to build the model is now explained. For better understanding, this procedure is summarized in the block diagram of Figure 3.3.

After being collected (step I) and processed (step II), data needs to be sorted into matrices (step III). The first three matrices to be generated are the base map, the profiles map and the conversion map no. 1.



Figure 3.3. Block diagram that summarizes the procedure adopted to build the CO₂e model. The procedure is divided in four steps addressed in roman numbers (I, II, III, IV, V). Consecutive steps are delimited by an horizontal dashed line. Matrices and their size are indicated within boxes.

The base map has 110 elements on each page, resulting from the product of 5 rows times 22 columns (categories of consumption times categories of use). Each element of the base map is a number that indicates the specific consumption of an energy vector (or a carbonate) per tonne of glass or per hour of production, for a specific use. For instance, element (1,4) contains information on the specific gas consumption of the oven (column 4) per tonne of flat glass pulled out of the oven (row 1). Element (2,6) contains information on the specific diathermic oil consumption assembly laminate (column 6) per tonne of laminated produced (row 2).

The information about the specific consumptions of each category of use was calculated by dividing the annual consumption by tonne of glass or hour of production. The annual consumptions of each category, in turn, was calculated starting from the estimation of the consumption of each single device. Eventually, the calculation was compared with real data read on gas meters and electricity meters. Moreover, during this step two important maps are generated: the profile map and the conversion map no. 1. The profile map contains both production schedule and time schedule that describe when and how much the plant produced in 2018. Schedules are precisely arranged in the profile map beacuse they have to match with the particular combination of category of use and consumption that they are describing. The conversion map follows the same principle: it contains conversion factors from secondary energy vectors to primary energy vectors and they are arranged specifically to match positions with the base map and all the other maps.

The fourth step (IV) is the product between the base map, the profile map and the conversion map no. 1. The result of the calculation is the primary map. Each element of the primary map describes the hourly consumption of an energy vector or process input. Thanks to the conversion factors contained in the conversion map no. 1, all the secondary energy vectors are converted back to their primary energy vectors. This way, the primary map only contains electricity, gas, diesel and carbonates consumptions.

Before proceeding to the last step it is necessary to generate another conversion map. The conversion map no. 2 contains emission factors that allow to convert primary energy vectors and tonne of carbonates into tonne of CO_2e . This map has to match positions with the base map, as the previous ones.

The fifth step (V) is the product between the primary map and the conversion map no. 2. The map of hourly emissions of CO_2e is obtained. We will be reffering to this map as CO_2e map.

3.2.3 Emission factors

The emission factors adopted in this application are found in the literature. Since both ETS and ISO 14064 rely on the emission factors published in the IPCC 2006 Guidelines, there is no conflict between the two. The value of the emission factors used in this case study are listed in Table 3.1.

The emission factor of electricity consumed in the glass factory comes from the Italian electricity grid. The emission factor proposed in Table 3.2 for electricity refers to the electricity mix of the Italian electricity grid associated with gross electricity generation. The latest statistics on the gross electricity mix generation for Italy is provided by the European Enviroment Agency and refers to 2016. As it was not possible to find reliable 2018 data, the 2016 data is used instead. By the way, it is noted that the carbon intensity of gross electricity generation in Italy is decreasing steadily and it is below the European average since 2008 (see Appendix A, Figure A.3).

	EF	UM
Soda	0.415	t CO ₂ e / t soda
Limestone	0.44	t CO ₂ e / t limestone
Dolomite	0.239	t CO ₂ e / t dolomite
Gas	56.1	t CO ₂ e / TJ
Electricity	$2.562 \cdot 10^{-4}$	t CO ₂ e / kWh
Diesel	69.3	t CO ₂ e / TJ

Table 3.1. Emission factors used in this particular case study. Emission factors convert the usage of the energy vectors and process inputs into the respective volume of CO_2e .

3.3 Simulation results

The result of the procedure described in the previous paragraphs is a series of maps that contains important information. With the help of the graphical analysis it is possible to visualize the results of the simulation and draw conclusions on the case study and on the method itself.

Before generating any graph it is advisable to check for errors in the calculation. Therefore, the expected overall consumption of gas and electricity and the total volume of emissions predicted from the model has to be compared with the real data of 2018. To extract gas and electricity data from the model it is necessary to sum, along the three directions, all the elements belonging to the same energy vector in the primary map. To extract the overall emission data it is necessary to sum, along the three directions, all the elements in the CO_2e map. This comparison criterion alone does not guarantee that the model is correct, but it is a good start to check for errors in the script (i.e. the implementation of the model).

The values predicted by the model and the real data are compared in Table 3.2.

By looking at the relative error between real data and model results it can be concluded that the model is well calibrated, at least on a yearly basis. Energy consumption relative errors are around 1 percent, while the relative error on emissions reaches 5 percent. This incosistency is due to the fact that the glass factory relies on external laboratory tests for carbonates emissions factors while this thesis used standard emission factors obtained from the literature of the ETS and the ISO 14064. Moreover, the glass factory has access to the energy content of the gas supply, while this thesis used a standard calorific value obtained from ETS and ISO 14064 literature.

Once the yearly balance is checked, it is interesting to visualize how good is the model prediction on a tighter time detail. For this reason, the comparison between real and model data on daily consumptions of energy (gas, electricity) is provided in Figure 3.4, Figure 3.5 and Figure 3.6. In order for the data to be comparable, they have to be expressed in the same time frequency. Since real data is available only a daily basis while model data is on an hourly basis, it was necessary to calculate the daily average of the model data. This way,

Table 3.2. Overall 2018 data comparison between real values and model results on energy consumptions and co2e amissions. Real data was supplied directly by the installation, model data are obtained by calibrating the general CO_2e model on the specific installation, as described in this chapter. The last column indicates the relative error of the model with respect to the real data.

	Real data	Model results	UM	Error
Gas consumption	44'250'112	44'691'707	smc	+0.99%
Electricity consumption	30'564'536	31'019'829	kWh	+1.48%
CO ₂ e emissions (ETS)	128'006	121'684	ton CO_2e	-5%

both data are expressed on a daily basis.

Looking at Figure 3.4, an unusual behaviour is noticeable at the beginning of May. This evident drop in consumptions in May is due to a planned ordinary maintenance, that is done once every 7 years. During the maintenance, the production of flat glass stopped for a few hours to allow the replacement of the spout lip that connects the furnace to the tin bath. This lip is made of α/β Al₂O₃ and it is inevitably subjected to corrosion. During this operation, the oven continued to heat the glass mixture but a minimum amount of gas was burned because the supply of raw materials was interrupted. Meanwhile, the tin bath and the glass ribbon were kept in the liquid state by delivering extra power to the resistances over them. Contextually, the electricity consumption in this specific event increased significantly, as can be seen in Figure 3.6.

Since the maintenance operation improved the oven performances, the specific consumption of gas in the oven (category of use 4, category of consumption 1) was modelled using two different average values for the periods preceding and succeding the maintenance. The model that used two different specific consumption was called "new model" while the model that used only one specific consumption was called "old model". The difference between the performances of the two models can be seen by comparing Figure 3.4 and Figure 3.5. The results of the new model (green) are quite satisfactory while the old model (red) has a visible offset with respect to real data.

The same good result was not obtained for electricity profiles, which are depicted in Figure 3.6. Due to the high variability of the energy usage, it is difficult to precisely model the power absorption of each machinery, even on a daily basis.

Part of the electricity consumption is related to the tonne of flat glass pulled out of the oven. Since the production is suspended for a few hours during the maintenance event, the model predicts a negative spike. In reality, electricity consumption has a positive spike because extra resistances are turned on to keep the glass in a liquid state in the tunnel.

Still, the model profile (red) predicts electricity consumption in a conservative way, by flattening out the fluctuations of the real consumption data (blue).



Figure 3.4. Comparison between real and model data on the overall amount of gas consumed daily in the installation, in standard cubic meters. Real gas consumptions in blue, gas consumptions predicted by the new model in green.



Figure 3.5. Comparison between real and model data on the overall amount of gas consumed daily in the installation, in standard cubic meters. Real gas consumptions in blue, gas consumptions predicted by the old model in red.



Figure 3.6. Comparison between real and model data on the overall amount of electricity consumed daily in the installation, in kWh. Real electricity consumptions in blue, model predicted electricity consumptions in red.



Figure 3.7. ton of CO_2e emitted hourly by the glass factory in 2018, divided by sources. CO_2e from imported electricity in blue, CO_2e from gas combustion in red and CO_2e from carbonates in yellow.

Then, it is interesting to visualize the hourly emissions of CO_2e of the enrire installation, divided by sources (Figure 3.7). It is recalled that the ETS policy requires to account for combustion emissions (red) and process emissions (yellow) while the ISO 14046 requires to account also for the indirect energy emissions, which in this case is represented by electricity (blue). The largest quantity of CO_2e comes from the combustion of gas, which is mainly used to heat the oven.

Carbonates are the second source of CO_2e in the installation, followed by electricity. The CO_2e profiles of Figure 3.7 are very similar to the energy profiles predicted by the model in Figure 3.4 and 3.6 because energy and emissions are simply correlated through a conversion factor. Therefore, the maintenance event of may is very pronounced in the CO_2e profiles in Figure 3.7, too.

Another useful analysis is the discrimination of the emission volumes between categories of use (Figure 3.8). This analysis allows to classify and identify the most carbon intensive activities inside the glass factory. Additionally, it is particularly useful as a starting point for an improvement plan involving energy and process efficiency.

By looking at Figure 3.8 it is clear that the most carbon intensive category of use is the gas heating of the furnace. Indeed, more than 120'000 standard cubic meters of gas are burned every day. The volume of emission of this category is so high that it hinders the other entries on the histogram.

Figure 3.9 shows the contribution of each emission source in the total volume of emissions predicted by the model for 2018. It is seen that the larger volume of emissions is generated by the combustion of gas, which counts for two thirds of the total volume, followed by the use of carbonates (27%) and the consumption of imported electricity (6%).



Figure 3.8. Bar graph of the emission volumes in 2018 of the categories of use identified in the glass factory, in ton CO_2e . Each category is preceded by the primary energy vector from which it depends, with the exception of carbonates.



Figure 3.9. Cake diagram of the total 2018 emission volume predicted by the model, divided by source type. Emissions are expressed as percentage of the total amount of CO_2e .

Chapter 4

Economic Assessment

This chapter completes the study by introducing a techno-economic assessment on the potential short and long terms scenarios that could develop in the international carbon market established by the European Union. This assessment analyzes how process performances, energy prices and carbon allowance availability can affect the balance of the industrial installation analyzed in the previous chapter. Eventually, an economic risk assessment is performed by means of a Montecarlo Simulation.

4.1 Case scenarios

The subject of the techno-economic assessment is the glass factory described in the case study of chapter 3. The assessment is performed to evaluate how the yearly balance of an industrial installation can be influenced by variations in process efficiency, by fluctuations of the energy market and by fluctuations of the european carbon market. In particular, it is analyzed how the ratio between ETS emission costs and the sum of the energy and ETS emissions costs changes as a function of various inputs.

In total, four case scenarios were analyzed. Each scenario covers a 20-year period starting from 2018, and it is charachterized by the variation of different inputs.

The inputs of the case scenarios are electricity price, gas price, specific consumption of gas per tonne of flat glass pulled out of the oven, and percentage of free allocation of emission allowances. All the other variables, such as annual productivity, electricity consumption and carbonates consumption are kept constant. The reference year for the calculations is 2018, i.e. all the costs are discounted to this reference year. Each input is varied in a sensible range to study its effects on the outputs.

The outputs of the case scenarios are the tonnes of CO_2e emitted per year (in compliance with the ETS) and the cost ratio between the ETS allowance costs and the costs of energy and allowances, on a yearly basis. As specified in Equation 4.1, the energy and allowance costs are calculated as the sum of annual energy costs and ETS allowance costs. Raw material costs and other production costs are not considered.

$$cost \ ratio = \frac{allowance \ cost}{gas \ cost + electricity \ cost + allowance \ cost}$$
(4.1)

The characteristics of each simulated scenario are listed below.

1) The specific consumption of gas per ton of flat glass increases with a pace of 1% per

year (Case 1).

- 2) The specific consumption of gas per ton of flat glass increases with a pace of 1% per year and the energy price increases with a pace of 0.5% per year (Case 2).
- The specific consumption of gas per ton of flat glass increases with a pace of 1% per year and the price of carbon allowances increases with a pace of 0.5% per year (Case 3).
- 4) The specific consumption of gas per ton of flat glass increases with a pace of 1% per year and the percentage of free allocation decreases from year 11th with a pace of 2% per year (Case 4).

The pace of change of each input was chosen based on historical data. A detailed explanation of each pace of change is explained in the following paragraph.

The increase of the specific gas consumption is a consequence of the oven aging. According to the literature, a decay of 1% per year in the performances was found to be in line with experimental data on this type of ovens for glass manufacturing. Since the detetioration of the oven performances is inevitable, this input is common to all the case scenarios.

The energy price increase comprises both gas price and electricity price. Over the last 10 years, energy prices periodically fluctuated 20% above and below the mean value calculated on this past period (see Appendix A for details). Therefore it seemed reasonable to assume an increase at a 0.5% pace over the next 20 years.

The trend of carbon allowance prices is much more irregular compared to energy prices. From 2012 to 2017 the price of an allowance (i.e. the right to emit one tonne of CO_2e) ranged between a minimum of $3 \in$ to a maximum of $8 \in$. Since the beginning of 2018 the price have risen steadily until reaching $28 \in$ in July, 2019. Nowadays, the price settled around $25 \in$ per allowance. Therefore, it is difficult to foresee with a minimum confidence where the price will be heading to. It is commonly believed that this price settlement to $25 \in$ is permanent, at least for the forthcoming ETS phase 4 (2021-2030). As a cautionary measure, it is decided to increase the price of allowance at a pace of 0.5% per year.

The percentage of free allocation is the amount of allowances that each installation receives for free with respect to the total amount of allowances needed to cover all its emissions. The percentage of free allocation is calculated according to sector-specific benchmarks, so that installations that belong to the same sector (e.g. paper industry, iron industry, glass industry) have a similar percentage of free allocation. In the context of the 2030 climate and energy framework, EU leaders decided that over the next ETS period (2021-2030) the percentage of free allocation will remain unvaried, because a further decrease in free allocation would trigger carbon leakage. Carbon leakage is a situation in which, for reasons of costs related to climate policies, businesses transfer production to other countries with laxer emission constraints. The possibility of carbon leakage is highly discouraged by the European Union.

The downside of this issue is the fact that if the overall emission cost for installations does not rise, the shift towards low carbon technologies will be reiteratively postponed. For the reasons explained above, it is chosen to assume a decrease in percentage of free allocation only after the 11th year, with a pace of 2% per year.

The graphical representation of all case scenarios is reported in a plot of the outputs over the 20 year period (Figures 4.1 and 4.2).



Figure 4.1. *Output n.1 of the case scenarios analysis. Yearly volume of emissions in ton* CO_2e . The curves of the four case scenarios are overlapped.



Figure 4.2. *Output n.2 of the case scenarios analysis. Cost ratio between allowance cost and the sum of energy and allowance costs.*

Figure 4.1 displays the increase of the annual volume of emissions in ton CO_2e over the 20 year period. The curves of the four case scenarios are overlapped, as this output is influenced only by the specific consumption of gas per tonne of flat glass pulled out of the oven. Since

this input changes with the same pace for all case scenarios, the effects on the output will be the same in all the four cases.

Figure 4.2 displays the trend of the cost ratio over the 20 year period for all the case scenarios.

The cost ratio of case 1 (blue curve) slightly decreases from 4.26% to 4.18%, because the increase of the emission costs due to a higher volume of emissions is slower than the increase of the gas costs.

The cost ratio of case 2 (red curve) decreases from 4.26% to 3.8%, because the increase of energy costs due to a higher energy price makes the denominator of the cost ratio increase at a higher rate with respect to the nominator.

The cost ratio of case 3 (grey curve) slightly increases, from 4.26% to 4.60%, because the increase of the emission costs due to a higher allowance price and higher volume of emissions makes the numerator of the cost ratio increase at a higher rate with respect to the numerator.

The cost ratio of case 4 (yellow curve) is the same of curve 1 for the first ten years. After the 11th year, the percentage of free allocation starts to decrease and the cost ratio spikes rapidly. These results demonstrate how the percentage of free allocation is the variable that has the most impacting effect on the cost ratio. It should be noted that the intent of the EU is to bring the percentage of free allocation down to zero in order to pursue the long term objectives of a climate neutral Europe by 2050, which will therefore have a huge impact on the economical balance of industries.

4.2 Montecarlo Simulation Risk Assessment

Montecarlo Simulation (MCS) is a state-of-the-art methodology in risk analysis and finance. The MCS approach is one of the most popular stochastic optimization methods for risk management and strategic planning. MCS consists of an experiment that repeats a process or situation a large number of times, and generates a large number of random samples linked to specific variables. In order to apply MCS approach correctly, input variables have to be considered as independent random quantities, i.e. they must not be correlated to each other. As an industry benchmark, 10'000 iterations (N) are sufficient to obtain reliable, i.e. stable, results from MCS.

Urbanucci and Testi present the steps to perform MCS approach:

- A probability density function (pdf) has to be assigned to each input data x_i
- N possible values have to be generated for each input data, by means of random samples of its pdf
- The random samples have to be combined to get N input vectors
- The simulations of the model have to be performed N times, one for each input vector.

At this point, a vector of results is provided, and an input-output mapping of the model is defined. The set of the output data $(y_1, y_2 \dots y_N)$ defines the probability density function of the result of the simulation

In this specific application, MCS is performed to evaluate the economic risk that is linked to the future uncertainity of the carbon market. MCS is performed at the year 2038, i.e. the end of the 20-year period.

The inputs are the same of the previous case scenario analysis. They are electricity price, gas price, specific consumption of gas per tonne of flat glass pulled out of the oven and percentage of free allocation. All the inputs have a base-case 2038 value, which is calculated starting from 2018 and using the same pace of change reported in the case scenario analysis of the previous section. Therefore, 2038 values correspond to the values in the final year of the case scenario analysis. All the other variables, such as productivity, electricity consumption and carbonates consumption are kept constant to 2018 values. All costs are discounted to the reference year (2018).

The output (y_i) is the cost ratio between the CO₂e allowance cost and the energy and allowance costs, which is output n.2 of the previous case scenarios. For continuity, it will still be called output n.2 also in the following analysis.

They key aspect of MCS is to assign an appropriate probability distribution function (pdf) to the inputs. It is chosen to randomly vary the inputs in a bounded interval, so that all the N samples of each input have equal probability. The amplitude of each interval around the base-case 2038 value expresses the uncertainity (risk) related to that input.

The characteristics of each input of the MCS are summarized in Table 4.1.

Input	Base-case 2038 value	UM	Interval
Gas Price	0.32	€/smc	$\pm 25\%$
EE Price	0.1	€/kWh	$\pm 20\%$
Specific Consumption of Gas	223.8	smc/ton	$\pm 2\%$
Carbon Allowance Price	27.6	€/ton CO ₂ e	+20%
Percentage of Free Allocation	57	%	$\pm 35\%$

Table 4.1. Charachteristics of the inputs of the MCS risk analysis. Intervals are defined as increments or decrements of the base-case 2038 value.

The choice of each interval amplitude is explained hereafter.

Gas and electricity price intervals were directly related to the hystorical price fluctuations of the last ten years, as reported in Appendix A.

The interval of the specific consumption of gas is relatively small, as it is quite certain that oven performances decay by a certain extent over time.

Carbon allowance price range, unlike the rest of the input intervals, was defined as an increment-only type of interval because allowance auctions always have a bottom line price below which it is not possible to buy allowances.

The interval of free allocation was designed so that a minimum of 37% and a maximum of 77% are equally probable, which means that it is not excluded that the percentage of free allocation will remain unvaried to 2018 values (77%), even in 20 years time. Also, it is not excluded that the percentage of free allocation will drop to 37% as well.

All these input variables are varied iteratively for N=10000 times. The random generation of the value of the inputs was achieved by summing the base case 2038 value to the product between the base case 2038 value times the percentage range times a random number generated from the computer, rangin from -1 to +1. The only exception is represented by the carbon allowance price, because for this increment-only type of input the random number ranged from 0 to +1. At each iteration, the value of the cost ratio is reassessed.

The result of MCS is presented in the histogram of Figure 4.3. This histogram divides the N values of the cost ratio obtained from the MCS simulation into 10 classes of equal size. The cost ratio frequency curve (i.e. the fictional curve conecting the top of each bar) is normally distributed, meaning that the central values are those more frequent. The mean value of the cost ratio is 8.33%. The lowest value of the cost ratop is 3.54% while the highest value is 15.61%. The classes corresponding to a high or a low cost ratio are sparsely populated.

The cumulative percentage is the key indicator for risk assessment. By looking at the orange curve in Figure 4.3 and the corresponding Table 4.2 one can extract the following information: there is a 92% confidence that in 2038 the cost ratio will not exceed 11.76%. In other words, it is very likely that ETS emission costs will not exceed the 11.76% of the total energy and emisssion costs, on a yearly basis. In a decision making process, the lower the risk that an individual is willing to take, the higher is the corresponding cost ratio that is not exceeded. A detailed summary of the cumulative percentage data and frequency data is reported in Table 4.2.

Class	Frequency	Cumulative %
3.54%	0	0%
4.78%	478	4.78%
5.92%	1266	17.44%
7.00%	1522	32.66%
8.22%	1722	49.88%
9.45%	1786	67.74%
10.78%	1644	84.18%
11.76%	817	92.35%
13.00%	529	97.64%
13.85%	184	99.48%
15.61%	52	100%

Table 4.2. Classes, frequency and cumulative percentage of the cost ratio distribution

 resulting from MCS risk analysis.



Figure 4.3. *Histogram of the results of the MCS risk analysis. On the x-axis there are the classes of cost ratio. On the left abscyssa is reported the frequency of observation of cost ratio. On the right abscyssa is reported the cumulative percentage of cost ratio observations, which can also be read as the probability of not exceeding a specific class. The curve in orange that overlaps the graph is the cumulative percentage curve.*

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Conclusions

A model for the analysis and the prediction of greenhouse gases emissions of industrial installations has been successfully developed. The model complies with both the EU ETS and the ISO 14064, which are the two main aknowledged policies that provide guidelines to measure the impact of an installation in terms of greenhouse gas emissions.

The model, prior to a fine-tuning on the installation of interest, performs an accurate accounting of all the equivalent carbon dioxide emissions produced by the installation on a hourly basis. Moreover, thanks to the schematization of the model in the description of emissions, it is possible to recognize which activity has the greatest impact on the emission volume. This kind of information is useful to set up an improvement plan to reduce resource usage and decrease emission volumes, observing the concept of the Deming Cycle (Plan-Do-Check-act).

Another important feature of the model is its capacity to spot the drift from normal operating conditions. By comparison between predicted profiles and real data it is possible to spot deviations from regular marching operations and quantify performance losses in terms of carbon allowances. The extensive acquisition of real data requires the installation of transmitters and data loggers on the supply lines of the installation. This apparatus is becoming more and more popular between installations that monitor their energy usage and emission volumes, to prevent losses and commit to sustainability.

A case study performed on a glass factory, located in San Giorgio di Nogaro (UD) in Italy, allowed to validate the model and to make other interesting observations. The application of the model to the specific installation gave good results. The comparison between real and predicted gas consumptions highlighted how the maintenance intevention improved the oven performances. The comparison between real and predicted electricity consumptions was instead not satisfactory, due to the high variability of power absorption of each machinery within the installation boundaries. Still, the annual amounts of gas consumption, electricity consumption and emissions predicted from the model matched with the real data provided by the installation. According to the model, the activity with the greatest impact on the total emission volume was the combustion of gas in the furnace, which produced 86553 ton CO_2e over the year 2018. Moreover, the model allowed to calculate the role of each emission source on the overall 2018 emission volume: gas combustion emissions accounted for 67%, carbonates process emissions for 27% and imported electricity for 6%.

Thanks to a techno-economic assessment, it was seen that process performances, energy prices and availability of carbon allowances have an impact on the analyzed outputs, over a long term scenario. In particular, the percentage of free allocation was recognized as the input that has the highest impact on the allowance cost ratio, i.e the ratio between allowance

cost and the sum of energy and allowance costs. The Montecarlo Simulation provided a useful tool for decision making: using appropriate assumptions, it was found out that in 2038 it is very likely, with a 92% confidence, that the allowance cost will not exceed 11.76% of the total energy and allowance cost.

Nomenclature

AD = activity data (tonne or Nm³) AD_s = specific activity data (tonne/tonne or tonne/hour) CC = carbon content (-) CF = conversion factor (units of primary energy vector/units of secondary energy vector or tCO₂e/units of primary energy vector) CoF = conversion factor (-) EC = energy content (TJ) EF = emission factor (tCO₂/TJ or tCO₂/t or tCO₂/Nm³) EM_c = Combustion Emissions EM_p = Process Emissions FQ = fuel quantity (tonne or Nm³) NCV = lower calorific value (TJ/tonne ot TJ/Nm³) OF = oxidation factor (-) SCH = scheduled time production (-) SP = specific consumption of energy (energy/time or energy/tonne)

Acronyms

AER = Annual Emission Report EDGAR = Emission Database for Global Atmospheric Research EE = ElectricityETS = Emission Trading System GHG = Greenhouse Gas GWP = Global Warming Potential IPCC = Intergovernmental Panel on Climate Change ISO = International Standard Organization LULUCF = Land Use, Land Use Change and Forestry MCS= Montecarlo Simulation MRR = Monitoring and Reporting Regulation MRV = Monitoring, Reporting and Verification pdf = probability distribution function SAR = Second Assessment Report UM = Unit of measurement UNFCCC = United Nations Framework Convention for Climate Change

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Appendix A



Figure A.1. *Historical price of methane gas in Italy for non household consumers, taxes and levies excluded. These prices are valid for a range of annual gas consumption between 1'000'000 GJ and 4'000'000 GJ, which roughly corresponds to a consumption range between 28'000'000 smc and 114'000'000 smc. The horizontal dashed line corresponds to the mean value of gas price over the period 2007a-2019a. The coloured markers correspond to the highest (red) price and the lowest (green) price over the period analyzed. Near each marker it is indicated the percentage of deviation from the mean value. Source: Eurostat*



Figure A.2. *Historical price of electricity in Italy for non household consumers, taxes and levies excluded. These prices are valid for a range of annual electricity consumption between 20'000 MWh and 70'000 MWh. The horizontal dashed line corresponds to the mean value of electricity price over the period 2010b-2019a. The coloured markers correspond to the highest (red) price and the lowest (green) price registered over the reference period. Near each marker it is indicated the percentage of deviation from the mean value. Source: Eurostat*



Figure A.3. *Historical value of carbon intensity expressed as the quantity of* CO_2 *that is emitted to produce one kWh of electricity in Italy (red) and in Europe (green) from 1990 to 2016. Source: eea.europa.eu*
Appendix B

Matlab code model_sisecam_v02.m

```
clc
clear all
format long
close all
set(0,'DefaultLineLineWidth',1.5)
%% PRODUCTION SCHEDULE %%
cavato365=xlsread('matlabdata.xlsx','B1:B366');
lam365=xlsread('matlabdata.xlsx','J2:J366');
hourly=datetime(2018,1,1,0,0,0):hours:datetime(2018,12,31,23,0,0);
daily=datetime(2018,1,1,0,0,0):hours(24):datetime(2018,12,31,23,0,0);
prod_lam=[]; % array initialization
prod_float=[]; % array initialization
for i=1:length(cavato365)
prod_float=[prod_float,repmat(cavato365(i)./24,1,24)]; % float production
profile [t float/hour]
end
for j=1:length(lam365)
prod_lam=[prod_lam,repmat(lam365(j)./24,1,24)]; % laminate production
profile [t laminate/hour]
end
%% TIME SCHEDULE %%
h12=[1 1 1 1 1 1 0 0 0 0 0 0 0 0 0 0 0 1 1 1 1 1 1 ]; % 1=on, 0=off
h4=[0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 1 1 0 0 0 0 0 0 0 0 ]; % 1=on, 0=off
sch_lam_2018=[ riposo repmat(h24,1,216) repmat(riposo,1,16)
repmat(h24,1,123) repmat(riposo,1,9)]; % laminate time schedule
sch_float_2018=[repmat(h24,1,365)]; % float time schedule
sch_night_2018=[repmat(h12,1,365)]; % night lightining time schedule
AC=[repmat(h4,1,6) riposo]; % air conditioning weekly time schedule
sch_win_2018=[repmat(AC,1,9) repmat(riposo,1,302)]; % wintern heating time
schedule
```

```
sch_sum_2018=[repmat(riposo,1,154) repmat(AC,1,12) repmat(riposo,1,127)];
% summer cooling time schedule
%% BASE MAP %% [secondary energy vectors] %% 5x22
UO_Na=[0.1933; 0; 0; 0; 0]; % t Na2CO3/t float
U0_Ca=[0.0641; 0; 0; 0; 0]; % t CaCO3/t float
U0_MgCa=[0.1407; 0; 0; 0; 0]; % t MgCa(CO3)2/t float
U1=[183.427; 0; 0; 0; 0]; % smc gas/t float
U2=[0.2135; 0; 0; 0; 0]; % kWht/t float
U3=[0; 50.5152; 0; 0; 0]; % kWht/t lam
U4=[1.7748; 0; 0; 0; 0]; % kWh/t float
U5=[22.6719; 9.4723; 0; 0; 0]; % kWh/t float & kWh/t lam
U6=[3.1955; 0; 0; 0; 0];% kWh/t float
U7=[7.3986; 1.6948; 0; 158.6001; 0]; % kWh/t float & kWh/t lam & kWh/h
float & kWh/h lam & kWh/h
U8=[14.7816; 36.1815; 0; 0; 0;]; % kWh/t float & kWh/t lam
U9=[3.5404; 0; 0; 0; 0;]; % kWh/t float
U10=[67.2004; 119.7093; 0; 0; 0;]; % Nmc aria/t float & Nmc aria/t lam
U11=[9.7927; 0; 0; 0; 0;]; % kWh/t float
U12=[23.2580; 0; 0; 0; 0; 0;]; % kWh/t float
U13=[0; 0; 5.065; 0; 0]; % kWh/t float
U14=[0; 0; 0; 0; 0; ];
U15=[0; 0; 0; 0; 239.53;]; % kWh/h % wintern heating
U16=[0; 0; 0; 0; 256.87;]; % kWh/h % summer cooling
U17=[0; 0; 124.1784; 25.446; 123.3555]; %kWh/h internal lightning 8760
U18=[0; 0; 0; 0; 19.0342]; %kwh/h external lightning 4380
U19=[0; 0; 0; 0; 13.0023]; %kwh/h % small electrical devices 8760
map0=[U0_Na U0_Ca U0_MgCa U1 U2 U3 U4 U5 U6 U7 U8 U9 U10 U11 U12 U13 U14
U15 U16 U17 U18 U19]; % 2D base map
%% THIRD DIMENSION PROJECTION OF THE 2D BASE MAP %% 5x22x8760
for i=1:length(sch_lam_2018)
map2(:,:,i)=map0(:,:);
end
map2(1,4,:)=permute([repmat( 188.381,1,3048) repmat(619.4792901,1,48)
repmat( 180.444,1,5664)],[1 3 2]);
%% PROFILES MAP %% 5x22x8760 %% COMBINATION OF PRODUCTION SCHEDULE AND
TIME SCHEDULE %%
profile_map=[repmat(permute(prod_float, [1 3 2]), 1, 22);
```

repmat(permute(prod_lam,[1 3 2]),1,22);

```
repmat(permute(sch_float_2018, [1 3 2]),1,22);repmat(permute(sch_float_2018,
[1 3 2]),1,10) repmat(permute(sch_lam_2018,[1 3 2]),1,12);
repmat(1,1,17,8760) permute(sch_win_2018,[1 3 2]) permute(sch_sum_2018,[1
3 2]) permute(sch_float_2018, [1 3 2]) permute(sch_night_2018, [1 3 2])
permute(sch_float_2018,[1 3 2])];
%% CONVERISION MAPs %% 5x22x8760
boiler_efficiency=0.93;
NCV_gas=9.685; % kWh/smc compressor_efficiency=[0.1 ; 0.08];
secondary_to_primary=[repmat(1,1,4,8760) repmat(1/boiler_efficiency/NCV_gas,
1,1,8760) repmat(1,1,7,8760) repmat(0.1,1,1,8760) repmat(1,1,9,8760);
repmat(1,1,5,8760) repmat(1/boiler_efficiency/NCV_gas,1,1,8760)
repmat(1,1,6,8760) repmat(0.08,1,1,8760) repmat(1,1,9,8760);
repmat(1,1,22,8760); repmat(1,1,22,8760); repmat(1,1,22,8760)];
carbonate_EF=[0.415 0.440 0.239]; % carbonate emission factor [tC02 / t
carbonate]
gas_EF=[1.955967/1000]; % gas combustion emission factor [tCO2 / smc gas
IPCC 2006]
electricity_EF=[0.2562/1000]; % italian electricity emission factor [tC02
/ kWh]
primary_to_CO2=[repmat(carbonate_EF,1,1,8760) repmat(gas_EF,1,3,8760)
repmat(electricity_EF,1,16,8760); repmat(1,1,5,8760)
repmat(gas_EF,1,1,8760) repmat(1,1,1,8760) repmat(electricity_EF,1,15,8760);
repmat(electricity_EF,1,22,8760); repmat(electricity_EF,1,22,8760);
repmat(electricity_EF,1,22,8760)];
%% PRIMARY MAP = base map * conversion map n.1 * profiles map %%
map1=map2.*secondary_to_primary.*profile_map;
%% CO2 MAP = primary map * conversion map n.2 %%
mapCO2=map1.*primary_to_CO2;
%% PLOTS AND CALCULATION CHECK %% carbonates=map1(1,[1:3],:);
gas_float=map1(1,4,:);
gas=map1([1:2],[4:6],:);
electricity=map1(:,[7:22],:);
EE_model_hourly=permute(sum(sum(electricity,1),2),[1 3 2]); % total
consumption of electricity per hour % kWh/hour
gas_model_hourly=permute(sum(sum(gas,1),2),[1 3 2]); % total consumption
of gas per hour % smc/hour
CO2_tot=sum(sum(mapCO2,1),3);
CO2_ETS=sum(CO2_tot(1,[1:6]));
```

```
figure(1)
subplot(1,2,1)
plot(hourly,permute(gas_float,[1 3 2]))
title('Hourly consumption of gas in the furnace')
xlabel('Months')
ylabel('m3/hour')
subplot(1,2,2) plot(hourly,permute(mapCO2(1,4,:),[1 3 2]))
title('Hourly emission of CO2 from gas combustion in the furnace')
xlabel('Months')
ylabel('t CO_2/hour')
figure(2)
plot(hourly,gas_model_hourly)
title('Hourly consumption of gas in the plant')
xlabel('Months')
ylabel('m3/hour')
figure(3)
plot(hourly,EE_model_hourly)
title('Hourly consumption of electricity in the plant')
xlabel('Months')
ylabel('kWh/hour')
figure(4) %CO2 comparison
plot(hourly,permute(sum(sum(mapCO2(:,[7:22],:),
1),2),[1 3 2]))
title('Hourly emission of CO_2e')
hold on
plot(hourly,permute(sum(sum(mapCO2(:,[4:6],:),1),2),[1 3 2]))
plot(hourly,permute(sum(sum(mapCO2(:,[1:3],:),1),2),[1 3 2]))
legend('imported electricity','gas combustion','carbonates')
set(xlabel('Months'),'FontSize',12);
set(ylabel('t CO_2/hour'),'FontSize',12);
%% COMPARISON WITH REAL DATA %%
EE365=xlsread('matlab_data.xlsx','E1:E366'); % kWh/day
gas365kwh=xlsread('matlab_data.xlsx','F2:F366'); %kwh/day
gas365=xlsread('matlab_data.xlsx','G2:G366'); %smc/day
gas12=xlsread('matlab_data.xlsx','M2:M13');
gas_model_1=sum(reshape(gas_model_hourly,24,365));
EE_model_daily=sum(reshape(EE_model_hourly,24,365)); % kWh/day
EE365_float=xlsread('matlab_data.xlsx','D2:D366');
```

```
EE365_lam=xlsread('matlab_data.xlsx','C2:C366');
EE12=xlsread('matlab_data.xlsx','L2:L13');
meanEE=[repmat(EE12(1,1)./31,1,31) repmat(EE12(2,1)./28,1,28)
repmat(EE12(3,1)./31,1,31)...
repmat(EE12(4,1)./30,1,30) repmat(EE12(5,1)./31,1,31)
repmat(EE12(6,1)./30,1,30) ...
repmat(EE12(7,1)./31,1,31) repmat(EE12(8,1)./31,1,31)
repmat(EE12(9,1)./30,1,30) ...
repmat(EE12(10,1)./31,1,31) repmat(EE12(11,1)./30,1,30)
repmat(EE12(12,1)./31,1,31)];
meanEE_model=[sum(EE_model_daily(1,[1:31])) sum(EE_model_daily(1,[32:59]))
sum(EE_model_daily(1,[60:90]))...
sum(EE_model_daily(1,[91:120])) sum(EE_model_daily(1,[121:151]))
sum(EE_model_daily(1,[152:181]))...
sum(EE_model_daily(1,[182:212])) sum(EE_model_daily(1,[213:243]))
sum(EE_model_daily(1,[244:273]))...
sum(EE_model_daily(1,[274:304])) sum(EE_model_daily(1,[305:334]))
sum(EE_model_daily(1,[335:365]))]';
EE_comparison=[EE12 meanEE_model (EE12-meanEE_model)./EE12.*100; sum(EE12)
sum(meanEE_model) ...
(sum(EE12)-sum(meanEE_model))./sum(EE12).*100];
meangas_model=[sum(gas_model_1(1,[1:31])) sum(gas_model_1(1,[32:59]))
sum(gas_model_1(1,[60:90]))...
sum(gas_model_1(1,[91:120])) sum(gas_model_1(1,[121:151]))
sum(gas_model_1(1,[152:181]))...
sum(gas_model_1(1,[182:212])) sum(gas_model_1(1,[213:243]))
sum(gas_model_1(1,[244:273]))...
sum(gas_model_1(1,[274:304])) sum(gas_model_1(1,[305:334]))
sum(gas_model_1(1,[335:365]))]';
gas_comparison=[gas12 meangas_model (gas12-meangas_model)./gas12.*100;
sum(gas12) sum(meangas_model) (sum(gas12)-sum(meangas_model))./sum(gas12)
.*100];
figure(5) % electricity comparison
plot(daily,EE365)
hold on
plot(daily,EE_model_daily)
title('Global electricity consumption per day')
set(xlabel('Months'),'FontSize',12);
```

set(ylabel('kWh/day'),'FontSize',12);

```
legend('real', 'model')
figure(6) % gas comparison
plot(daily,gas365)
hold on
plot(daily, gas_model_1)
title('Global gas consumption per day') legend('real', 'model')
set(xlabel('Months'), 'FontSize', 12);
set(ylabel('smc/day'), 'FontSize', 12);
hold off
```