External Costs as a Tool to Promote Short-Sea-Shipping

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Thesis to obtain the Master of Science Degree in

Naval Architecture and Ocean Engineering

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November 2022

TÉCNICO LISBOA

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DECLARATION:

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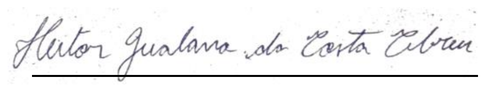

ACKNOWLEDGMENTS:

I hereby express my gratitude to my family in Brazil, Eliane, Marcelo, Manoela, and Mauro, and my family in Portugal, João and Maria Antónia, who kindly welcomed me in this stage of my life. My gratitude also to Professor Tiago Santos for believing in my work and allowing me to contribute to such an important research topic. Finally, I would like to thank Pedro Martins for his contribution in developing the models of the transport network and intermodal chains.

ABSTRACT:

The dissertation comprises, firstly, a literature review on emissions methods and external costs of transportation. The focus will be the evaluation of the competitiveness of waterborne transportation. A review of externalities internalization levels for the different transport modes in European Union was included by reviewing current greenhouse gases and other policies established by IMO and the European Commission. The new version of the software Sustainability Analyst includes the habitat damage costs. The software calculates external costs for varying numbers of transport chains for different pairs origin-destination, identifying possible transport chains for a specific destination. The results of emissions and external costs computed are validated by using alternative software and online calculators, even if the websites available are limited.

The software is applied to study several scenarios: current and expanded scope of intermodal routes over uncertainties about cargo utilization factor; Diesel and Electric freight railway service in operation in the Atlantic corridor; and expanded Short-Sea-Shipping service to the West Mediterranean. A comprehensive set of maps is developed to illustrate the regional preferences as regards different alternative transport chains and modal splits estimated for multiple pairs of Portugal-NUTS2 under different scenarios. An increased cargo utilization factor reduced external cost in the preferable route by 22% and the adoption of new intermodal routes represented a reduction of external costs by 20%. By computing also internal costs, external costs are shown to be only 29% of the total cost, limiting the increase in the competitiveness of intermodal routes related to a better environmental performance.

Keywords:

Short sea shipping, Intermodal transport, Maritime transport, Emissions, External Cost.

RESUMO:

A dissertação compreende, primeiramente, uma revisão de literatura sobre métodos para avaliação de emissões e custos externos do transporte. O foco será a avaliação da competitividade de modais aquaviários. Uma revisão dos níveis atuais de internalização de custos externos para diferentes países da União Europeia foi incluída pela revisão de políticas de abatimento gases do efeito estufa e outras externalidade estabelecidos pela IMO e Comissão Europeia. A nova versão do software calcula custos externos para um número variado de cadeias de transportes para diferentes pares origem-destino, identificando caminhos possíveis para destinos específicos. Os resultados de emissão e custos externos calculados são validados usando um software alternativo e calculadoras online, mesmo que estes sejam limitados.

O software é aplicado ao estudo de diferentes cenários: escopo de rotas intermodais atual e expandido sobre incertezas do fator de utilização de carga; serviço de afretamento ferroviário a propulsão Diesel e elétrica em operação no corredor Atlântico; e rotas de curta navegação no oeste do Mediterrâneo expandidas. Um abrangente conjunto de mapas é desenvolvido para ilustrar a preferência regional com relação a diferentes alternativas de cadeias de transporte e divisão modal estimada para múltiplos pares de Portugal-NUTS sobre diferentes cenários. O aumento da utilização da capacidade de carga reduziu custos externos em 22% e a adoção de novas rotas intermodais apresentou redução de 20% das externalidades. Após calcular os custos internos, os custos externos apresentaram-se como sendo 29% dos custos internos do transporte, limitando a competitividade de rotas intermodais relacionados com o melhor desempenho ambiental.

Palavras-chave:

Transporte Marítimo de Curta Distância, Transporte Intermodal, Transporte Marítimo, Emissões, Custos externos.

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ACRONYMS:

AIS: Automatic Identification System

CO: Carbon Monoxide

CO_2: Carbon Dioxide

CO_2: Carbon Dioxide Equivalent

CH_4: Methane

DPF: Diesel Particulate Filters

DS: Dry Scrubbing

DWT: Deadweight tonnage

EC: European Commission

EGR: Exhaust Gas Recirculation

EU: European Union

EUR: Euros

FEU: Forty-foot equivalent Transport Unit

GTW: Gross tonnage weight

HAM: Humid Motor Air System

HDV: Heavy-Duty Vehicles

HFO: Heavy Fuel Oil

IMO: International Maritime Organization

IWT: Inland waterways transportation

MCO: Maximum continuous output

MDO: Marine Diesel Oil

N_2O: Nitrous oxide

NOx: Nitrogen oxides

PM: Particulate matter

PTO: Power-Take Off

SECA: SO_X Emission Control Area

SO_X: Sulphur Oxides

SO_2: Sulphur dioxide

SSS: Short Sea Shipping

TEN-T: Trans-European Network

TEU: Twenty-foot equivalent Transport Unit

ULSFO: Ultra-Low Sulphur Fuel Oil

VLSFO: Very-Low Sulphur Fuel Oil

WIF: Water in fuel

WS: Wet Scrubbing

SYMBOLOGY:

$F_{I,ijk}$: truck inertial force, in N

M_{ij}: truck gross weight, in ton

V_{ijk}: link speed, in km/h

$F_{d,ijk}$: truck drag force resistance, in N

ρ_{air}: air density, in kg/m^3

C_d: drag coefficient

A_f: truck frontal area, in m^2

$F_{r,ij}$: truck rolling force, in N

C_{rr}: rolling coefficient

g: gravity acceleration, in m^2/s

θ: road gradient, in rad

$F_{g,ij}$: truck grade force, in N

$F_{T,ijk}$: total truck resistance force, in N

$P_{D,ijk}$: power demand, in kW

η_t: transmission efficiency

L_{ijk}: link length, in km

$EF_{e,p}$: energy-based emission factor, in g/kWh

$EF_{f,p}$: fuel-based emission factor, in g/g

$E_{ijk,p}$: air pollutant emissions, in g

SCF_{ij}: specific fuel consumption, in g/kWh

SC: fuel sulphur content, in ppm

EC_{ij}: energy consumption factor, in MJ/tkm

FC_{ij}: Fuel consumption, in kg/h

$FC_{ME,ij}$: main engine fuel consumption, in g

$FC_{ME,ij}^{sea}$: main engine fuel consumption at navigating profile, in g

$FC_{ME,ij}^{mano}$: main engine fuel consumption at maneuvering profile, in g

$P_{EF,ijk}$: effective power, in kW

L_{PTO}^{sea}: Power-Take Off load percentage

PTO_{ij}: total Power-Take Off capacity, in kW

$\delta\Delta_{ij}$: vessel's deadweight variation, in ton

DWT_{ij}: vessel's deadweight, in ton

W_{FEU}: estimated FEU weight, in ton

Cap_{ij}: vessel's capacity, in FEU

Ut_{ij}: cargo utilization factor

δD_{ij}: vessel's draft variation, in m

A_w: waterplane area, in m^2

γ: saltwater density, in kg/m^3

L_f: vessel's length at waterplane level, in m

B_f: vessel's breadth at waterplane level, in m

c_w: waterplane coefficient

$L_{PP_{ij}}$: length between perpendiculars, in m

B_{ij}: vessel's summed draft, in m

D'_{ij}: vessel's draft in actual cargo condition, in m

D_{ij}: vessel's summer draft, in m

PME_{ij}: installed main engine power at MCO, in kW

η_w: weather efficiency

η_f: fouling efficiency

SFC_{base}: main engine base specific fuel consumption, in g/kWh

$C_{AP,ijk}$: air pollution cost, in EUR

$C_{CC,ijk}$: climate change cost, in EUR

$C_{ext,ijk}$: external cost related to externality ext, in EUR

$c_{p,ijk}$: unit external cost related to pollutant p, in EUR/ton

K_r: regional transfer value

1. INTRODUCTION

1.1 Background and Motivation

Climate change is one of the main challenges for the humanity in the 21st century and one of its effects are extreme weather events. In fact, in July 2022, western Europe experienced temperatures ranging between 38°C and 40°C caused by a persistent heatwave in different regions of the continent. In France, the temperature reached 37.6°C on July 18th, the warmest day registered in the last 20 years (Le Monde, 2022); on the next day, climatologists recorded 40.3°C in the United Kingdom, the highest temperature ever reached in the country (BBC, 2022). During this month, extreme heat was associated with 1,700 deaths on the Iberian Peninsula (WHO, 2022), airport and railway service disruptions in the United Kingdom (The Guardian, 2022), droughts and wildfires spreading across Portugal, Greece, Spain, and Italy (BBC, 2022; RP, 2022).

Consistent climate action is required internationally to contain the advance of different consequences related to climate change, especially global warming. Action is required in all sectors of human activity, including transportation. The major culpable for the temperature rise are greenhouse gases (GHG), i.e., carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), and fluorinated gases (hydrofluorocarbons, perfluorocarbons, SF_6, and NF_3), also known as $CO_{2\text{-eq}}$ emissions (carbon dioxide equivalent). Its emissions are responsible for restricting the Sun's heat on the Earth's atmosphere, the so-called Greenhouse effect (EC, 2022). Although this is a natural phenomenon, human activity has accelerated the heating process due to excess emissions, leading to current extreme weather events. Nevertheless, other gases are also associated with harmful to human health and the environment and their emissions have also to be considered. The scientifically proved harmful gases are mainly sulphur oxides (SO_X), particulate matter (PM), and nitrogen oxides (NO_X) (EEA, 2021). For this reason, the reduction of the previously mentioned air pollutants and GHG emissions are the main drivers of local and international policies for containing climate change effects.

The 13th goal proposed by the United Nations (UN) for sustainable development establishes a call to action for national and international policies focused on environment protection, education, and mitigation measures based on the Paris Climate Agreement, signed by 192 member countries. Proposed at the UN Climate Change Conference (COP21) in 2015, the Agreement aims to reduce GHG emissions to contain the global temperature rise to 2°C above pre-industrial levels through a review of parties' commitment every 5 years and climate financing funds to developing countries (UN, 2022). As the third-largest emitter in the world, the European Union (EU) has also presented additional efforts to reduce emissions and achieve sustainable development. Besides UN climate targets, the European Commission (EC) proposed the European Green Deal in 2019, a core strategic plan to turn Europe into the first climate-neutral continent by 2050 (EC, 2019b). In July 2021, EC announced the 'Fit for 55', a package of proposals aiming to achieve the Green Deal purpose – net GHG emissions levels reduction not less than 55% compared to emission levels registered in 1990; at least 32% share of renewable energy; and 32.5% energy efficiency improvement by 2030. The actions have important implications in most economic sectors through new directives and financial endowment programs.

Regarding the source of emissions, GHG emissions analysis by economy sector showed that the transportation sector constitutes 14% of global emissions in 2010 (EPA, 2010). However, considering emissions in the EU, freight and passenger transport emission shares increased to 29% in 2018 (ICCT, 2019). The same source indicates that the road mode and marine transportation are responsible for 5% and 4% of total economy-wide emissions in 2018, respectively. It is evident the need for environmental regulations in the transportation sector for the sake of meeting the stated climate targets, covering all modes of transportation.

Therefore, the transportation sector is a key point of attention for the European Union to achieve its climate goals defined by the European Green Deal. In the next 5 years, the 'Fit for 55' package will affect the maritime sector through four different directives and regulations – the European Trading System (ETS) Directive, FuelEU Maritime Regulation, Alternative Fuels Infrastructure Regulation, and Energy Taxation Directive (DNV, 2021). The effort for the decarbonization of shipping in the EU has also implications for international navigation due to the economic union's extra-territorial trade and the short implementation time of such actions (Maersk, 2022).

By the EU-ETS Directive, shipping companies are allowed to emit a certain limit (cap) of CO_2 and, in case this limit is exceeded, it is possible to buy allowances or, in case emissions are lower than the cap, the company can trade its credits, which price fluctuates according to the market demand and supply of allowances. Over time, the cap is reduced allowing a reduction in total emissions. This measure will be partially introduced, allowing ships to handle 20% of the verified emissions in 2023 with a gradual percentage until the total reported emissions in 2026. The FuelEU Maritime Regulation, in addition, incentives the use of renewable and low-carbon fuels in ships (Hellenic Shipping News Worldwide, 2022c). Moreover, LNG bunker availability by 2025 and shore electrical supply by 2030, according to the Alternative Fuel Infrastructure Regulation, and taxation over the use of conventional fuels, according to the Energy Taxation Directive, are additional requirements introduced by the EU for shipping decarbonization.

On the other hand, vessels transport a large number of goods along large distances, allowing an economy of scale and increasing its sustainability importance in terms of carbon intensity compared to land-based modes. Although efforts for the decarbonization of the shipping industry contribute to sustainable development, some measures can negatively impact the sector by introducing more expensive fuels or taxations, which are translated to higher maritime freight rates. Consequently, modal shifts from maritime transport to road modal can have a negative effect on reducing emissions, considering that a more environmental-friendly mode is abandoned. Especially in Europe, Short-Sea-Shipping (SSS) can be affected by new regulations, with the possible shutting down of RoRo lines (Zis & Psaraftis, 2017).

A way to promote maritime transport is to apply Market-based Measures (MBM), in which the guiding philosophy is the "polluter pays" principle through external cost internalization. The concept of the external cost was developed by British economist Arthur Cecil Pigou (1877–1959) in his book *Economics of Welfare* and it is defined as "a cost or benefit that is imposed on a third party who has not agreed to incur that cost or benefit" (Pigou, 1920). Externalities from the transport sector can be monetized from different perspectives, however, when the range of negative effects is considered in an intermodal chain, including all different modes of transport, the external cost internalization can help in decision-making, allowing the identification of the route with lower environmental costs. Without full internalization, shipping companies are subjected to losing the competition to more polluting modes to cope with new environmental regulations and directives.

In April 2022, the European Commission approved €60 million in funding for encouraging Spanish maritime freight transport instead of using the road mode, through the Recover and Resilience Facility plan. The scheme involves direct grants to road haulers to move to SSS, motivated by the argument that external costs from transportation could be reduced by using maritime transport (EC, 2022b). Following the same fund program, the country has received €120 million in incentives for the railway transportation infrastructure (EC, 2022a) with the objective of promoting freight transport substitution. These are some examples of political efforts based on external costs for increasing sustainable modes of transportation competitiveness.

It is therefore clear from the above that it is important to base all analysis of emission reductions and modal shift policies on suitable numerical tools capable of assessing and comparing intermodal transport chains, on a door-to-door basis, including all modes of transportation, considering both internal and external costs of transportation, GHG emissions and air polluting emissions. This thesis contributes to the development of such numerical tool and presents results of a comprehensive case study.

1.2 Objectives

The main objective of this thesis is to assess the potential of external cost internalization for encouraging SSS in Europe and analyze the impact of new intermodal chains in the decision-making process, considering or not environmental issues. A previously implemented software, Sustainable Analyst (SA), for computing airborne emissions and external costs has received additional modifications, its capabilities were extended and a validation process using a different tool was carried out with the purpose of enhancing the usability and applicability of the software in different studies. The numerical tool was also adapted for running through multiple transport chains, covering a vast geographical scope with route number differentiation per pair origin-destination (O/D). An extensive literature review of modern emission calculation methods and regulations was also carried out to use the state of art of emission methods and consider all external cost classes. To properly represent the current transportation practices in Europe, a study took place for defining the most accurate technical characteristics of trucks, trains, barges, and ships, considering the differences in existing lines along the continent.

Once reviewed the technical aspects of the software, different scenarios were defined to evaluate which route option is preferable considering different criteria – the lowest external cost, internal cost, and total transport cost. By doing so, it is possible to draw conclusions regarding the competitiveness of intermodal transport chains' performance (containing SSS) in comparison with unimodal road transport. Summarizing, the objectives of this thesis are:

- Carry out software adaptation to a new transport network,
- Review emission calculation numerical methods,
- Update vehicle technical characteristics in European transport networks,
- Study external cost internalization,
- Evaluate SSS competitiveness before and after internalization,
- Evaluate intermodal transport chain environmental performance.

1.3 Structure of the Thesis

The thesis is organized into seven chapters. Chapter 1 is the introduction of the topic to be discussed the related background and including the goals and structure of the work. Chapter 2 contains the literature review concerning the state of art of emission calculation methods for each mode of transport and a review of external cost internalization. Chapter 3 details the methodology which forms the basis of the numerical tool applied to the study, followed by its validation using another numerical tool, as described in Chapter 4. Chapter 5 presents the case study in detail, in which the geographical scope and technical characteristics of the vehicles are given. The numerical results in such scenarios and for specific input parameters are presented in a brief discussion in Chapter 6. Chapter 7 indicates the main conclusions of this thesis and provides a set of recommendations for further work.

2. LITERATURE REVIEW

2.1 Air Pollutant Emission Factors

Air pollutant emissions methods are divided into primary methods - direct measurement at the source point - and secondary - emission factors, and modeling. Besides both approaches having advantages and disadvantages, the second method is more commonly applied due to its simplicity and availability (Fan, et al., 2018). Direct measurement offers the advantage of lesser uncertainty, but it takes longer and makes it more expensive, with the drawback that the source of emission is unknown. Emission factors are one of the most common methods to obtain input data for assessment studies, however increasing uncertainties arise from emissions deterioration over the useful life of the vehicles, emissions characteristics variation among identical engines, and the impact of cold and hot start engines (JCR, 2017).

Different dimensions are considered when evaluating air emissions using emission factors - the quantity and region of air emissions – and, for both dimensions, a bottom-up or a top-down approach can be used. A full top-down approach is applied when the total emissions are calculated without considering the characteristics of the single vehicle and are later geographically located and assigned to different vehicles. On the other hand, in a full bottom-up approach, air pollutants are computed in a specific position (Miola & Ciuffo, 2011). In this section, a literature review is carried out regarding emission estimation methods in different modes of transportation, covering the most common methods for computing emissions and air pollution legislation.

2.1.1 Emissions from land-based transportation

Emission factors from land-based transportation, i.e., rail and road modes of transportation, are at the center of discussion since trucks and locomotives are important contributors to GHG emissions and other air pollutants. Transport accounts for around a quarter of all energy-related GHG emissions in Europe (EC, 2016), and heavy-duty vehicles (HDV), i.e., motor vehicles with a technically permissible maximum laden mass over 3,500 kg, account for 6% of all emissions (EC, 2019). The deterioration of air quality, especially in urban areas, has motivated several studies to measure the actual airborne emissions from road mode and in smaller intensity rail mode.

Concerning GHG emissions, extensive literature can be found in (Clairotte, et al., 2020), presenting N_2O and CH_4 exhaust emission factors from L-category, light-duty, and heavy-duty vehicles based on measurements carried out in the Vehicle Emission Laboratory of the Joint Research Centre between 2009 and 2019 and in (Zhang, et al., 2021), in which Well-to-Wheel methodology was used to evaluate CO_2 equivalent emissions in the hybrid truck. A review of literature also presented in (Speirs, et al., 2020) concerns a transition from Diesel to natural gas fueled trucks in terms of GHG emissions and costs involved, and further pollution prevention and mitigation solutions can also be found in (Inkinen & Hämäläinen, 2020) for road freight-based trucks. More specifically, emission models for the estimation of Greenhouse Gas (GHG) emissions from truck operations in port terminals were evaluated (Konstantzos & Saharidis, 2018).

Including other air pollutants, PM, CO_2, and NO_X emission factors based on portable emissions measurement systems were investigated in (Dhital, et al., 2021) to investigate the effect of vehicle attributes, driving behavior, and road grade. The dispersion of PM produced by HDV fuel combustion, and the number of deaths attributed to the PM emitted were analyzed in (Teixeira, at al., 2020) in the Brazilian transport system, also evaluating the transition to LNG-fueled.

In this study, the emission factors correspond to standard limits and fuel quality regulations in practice nowadays in accordance with the geographical scope. Road and non-road regulations established by the European Commission on all fuels commercialized in Europe are referred as Euro I to VI standards for new heavy-duty diesel engines equipped with compression ignition or positive ignition natural gas or liquefied petroleum gas (LPG) engines.

Both truck engines and urban buses were originally regulated by Euro I in 1992 and followed by Euro II in 1996. In 1999, Directive 1999/96/EC introduced Euro III standards and later Euro IV/V standards in 2005/2008, which rules were voluntary and established tougher emission limitations for enhanced environmentally friendly vehicles (EEVs). However, through Directive 2001/27/EC, the European Commission prohibited in 2001 the use of emission "defeat devices" and "irrational" emission control strategies that degrade the efficiency of emission control systems when vehicles run in conditions lower than those reached during emission testing.

For Diesel engine trucks, (DieselNet, 2022a) summarizes the emission standards present in previously mentioned regulations in two different testing requirements - Steady-State Testing and Transient Testing. The air pollutants regulated are CO, HC, NO_X, PM, PN, and smoke, which limits for the first 4 pollutants are set in grams of pollutant per kWh, PN in kWh^{-1}, and smoke in m^{-1}. For fuel-based air pollutants, $CO_{2\text{-eq}}$ and SO_X emissions were obtained by using the sulphur content present in the Diesel fuel, which quality is also limited by the European Commission. The last specification in the EN590 standard was published in 2004, establishing sulphur limits of 50 ppm (Euro 4) and 10 ppm (Euro 5), as regulated by Directive 2003/17/EC. These rules are also observed in non-road applications, such as rail transportation.

Studies focused on the impact of intermodal rail/road transport chains on GHG emissions and other air pollutant emissions. Compared to only-road transportation, recent publications show rail transportation as a more environmental-friendly mode, e.g., (Heinold & Meisel, 2018; Heinold & Meisel, 2019; Pinto, Mistage, et al., 2018; Kiyota, et al., 2012; Craig et al., 2013; Tong, et al., 2021). The impact of increasing speed on greenhouse gas emissions in high-speed rail (HSR) lines has also concluded important contributions to emissions during construction and operation phases (Jiang, et al., 2021; Lee, et al., 2020). More generally, (Yuan & Frey, 2021) evaluated CO_2, CO, NOx, PM, and hydrocarbon emissions using a speed trajectory simulator, energy method, and emission method, calibrated with actual data. For PM emission in two train lines in Washington city, (Jaffe, et al., 2014) evaluate air quality through emission factors obtained from direct measures of diesel particulate matter and coal dust.

A review of estimation such methods for computing emissions from rail freight transportation was analyzed in (Heinold A., 2020), in which five GHG emission models were evaluated - two from the MEET project, ARTEMIS model, EcoTransIT World model, and Mesoscopic model. The study has concluded that for some relevant train parameters, such as the number of wagons, payloads per wagon, speed, distance, and the number of stops, GHG emission estimation (in gCO_2e/ton·km) just impact some of the tools tested.

Like road transportation, rail transportation emissions are regulated by directives and regulations from European Commission for engines used in new non-road mobile machinery (NRMM). Directive 97/68/EC and five amending Directives published between 2002 and 2012 defined Stage I–IV requirements for Diesel engines. Regulation 2016/1628, which replaces Directive 97/68/EC and its revisions, establishes emission criteria for all types of compression ignition (diesel) and positive ignition mobile nonroad engines starting with Stage V.

Specifically for rail traction engines above 130 kW, Stage III A, and III B standards have been adopted for the propulsion of railroad locomotives and railcars. Later, the regulation was expanded and simplified for the propulsion of rail locomotives and railcars of any power rating and any type of ignition in Stage V emission standards. The limits for rail transport for CO, HC, NO_X, and PM are summarized in (DieselNet, 2022b).

2.1.2 Emissions from waterborne transportation

Addressing international shipping needs, the International Maritime Organization (IMO) is a specialized agency of the UN with responsibility for the safety and security of shipping, but also maritime and atmospheric pollution prevention. Since 2018, IMO has been providing important contributions to the global fight against climate change in support of the UN Sustainable Development Goals (UN General Assembly, 2015). For instance, the Energy Efficiency Design Index (EEDI) required a minimum energy efficiency level per ton-mile for different sizes and types of ships with the adoption of amendments to Annex VI of the 1997 MARPOL Protocol, promoting the use of less polluting equipment and engines, and at the same time promoting savings in energy cost. However, the design requirement imposes a limit only for CO_2 emissions, disregarding air pollutant emissions responsible for human and environmental health hazards.

The mentioned EEDI restriction is an effort to contain pollution levels in the first stage of a ship's life cycle – the ship design. Finalized in June 2022, the 78th section of the Marine Environment Protection Committee (MEPC 78) established the guidelines for an energy efficiency measure related to the technical design of a ship in operation. The Energy Efficiency Existing Ship Index (EEXI) corresponds to the mass of CO_2 emissions per ship's capacity and speed and its approval will be required by the first periodical survey in 2023 (DNV, 2020). Like the EEDI principle, the attained index must be lower than a required EEXI, given to a specific ship type, capacity, and propulsion. As the action date approaches, shipowners assess EEXI calculations and provide important data for the evaluation of the actual shipping decarbonization situation (Hellenic Shipping News, 2022a).

Applied to all ships under the same Annex VI of MARPOL Protocol, the Ship Energy Efficiency Management Plan (SEEMP) propose ways to shipping companies to keep track of emission levels during the ship's operational phase considering cost aspects (IMO, 2020). An example of voluntary measure is the Energy Efficiency Operational Indicator (EEOI), given by the mass of CO_2 per transport work (IMO, 2009b). Transport work depends on the vessel type, for instance the number of TEUs in a container ship or the metric tonnes of the cargo carried in a dry cargo carrier over a certain period. From 2024, the Carbon Intensity Indicator (CII) calculation will be annually required for ships engaged in international transport over 5,000 GT and SEEMP Part III will be a document used to evaluate the shipowner plan to improve such indicator for the following three years (DNV, 2022). The enhanced document addresses the importance of management systems aiming to cut GHG emissions from shipping.

Additionally, the creation of Emission Control Areas (ECA) was also an important international effort for reducing airborne emissions from ships carried out by IMO over regulation 13 of MARPOL Annex VI. These zones designate sea areas in which the concentration of pollutants (sulphur oxides in the case of SECAs, or nitrogen oxides in the case of NECAs) is limited through regulations over the fuel quality used on board ships navigating inside ECAs. Nowadays, SECAs are distributed on the North American coast, Baltic Sea, North Sea, and the United States Caribbean Sea areas, limiting the fuels sulphur content to 0.1%. In June 2022, MEPC 78 approved the extension of SECA to the Mediterranean Sea, coming into action after December 2022. This measure is associated with significant reductions in sulphur oxides and particulate matter emissions, benefiting the air quality in coastal regions and ocean acidification (Hellenic Shipping News Worldwide, 2022b). In international waters outside ECA, the sulphur content is controlled since 2005, and the requirement constantly evolves. Since the first international limit established in 2005 to 4.5%, the sulphur content was reduced to in 2012 to 3.5% and a significant reduction to 0.5% came into force in 2020 under regulation 14.1.3 of MARPOL Annex VI (IMO, 2016), but still five times greater than inside ECA. Figure 1.1 presents the evolution of sulphur regulations by IMO in regions outside and inside ECA.

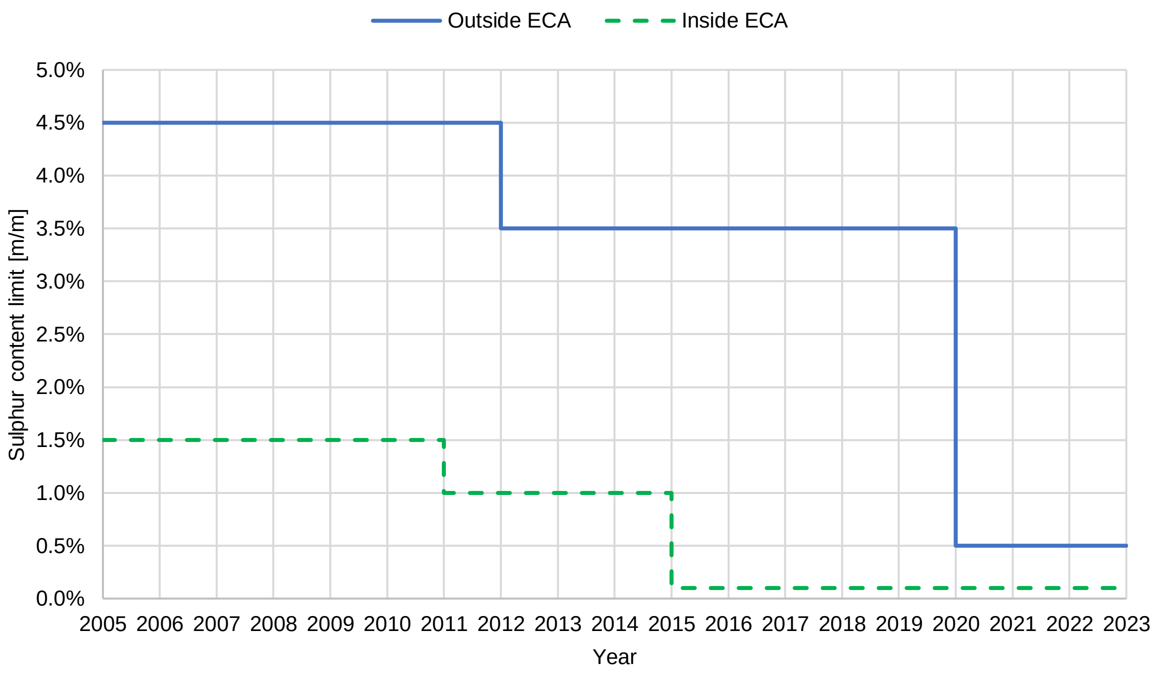


Figure 2.1 – Evolution of sulphur content limit in region inside and outside ECAs

The literature about ship emissions is extensive and it has been developed over several years. Early publications mainly focused on non-GHG gases can be found in (Bremnes, 1990) and global inventories of NO_X and SO_X emissions were analyzed by (Corbett, et al., 1999). Later, a bottom-up estimate of fuel consumption and vessel activity for international fleets was studied by (Corbett & Koehler, Updated emissions from ocean shipping, 2003) to address some uncertainties present in previous inventories related to fuel type used, and an update of marine emission inventories is proposed. A similar approach can be found in (Endresen, et al., 2003), who focused on global emission inventories of NO_X, SO_2, CO, CO_2, and VOC, and (Endresen, A historical reconstruction of ships' fuel consumption and emissions, 2007), who focused on fuel-based CO_2 and SO_2 inventories. Additionally, a historical review of emissions from international shipping was carried out by (Eyring, et al., 2005) and provides an emission inventory between 1950-2001 using ship and average engine statistics.

Among recent emission frameworks, the Ship Traffic Emissions Assessment Model (STEAM) is the method for evaluation of the exhaust emissions of marine traffic based on data provided by AIS and firstly described in (Jalkanen, et al., A modelling system for the exhaust emissions of marine traffic and its application in the Baltic Sea area, 2009) for the short-sea traffic in the Baltic Sea area. Further updates on the method can be found in (Jalkanen, et al., 2012), which presents PM and CO emission factors updates, and in (Johansson L., et al., 2013) with additional analysis on the effect of the new IMO regulation inside SECA in Europe. In its last version, a global assessment of shipping emissions in 2015 on a high spatial and temporal resolution is described in (Johansson, et al., 2017). The emission computation methodology can be used in any marine region in the world, if AIS data for that location is accessible and the method comprises the basis of current IMO emission computations regarding emission factors based on engine load use. Additionally, (Olmer, et al., 2017) have also published a detailed methodology for creating fuel-based inventories of global ship emissions.

Further literature reviews regarding emission factors in maritime transportation can be found in (Miola & Ciuffo, 2011), presenting a meta-analysis of research published until roughly 2011, and (Nunes, et al., 2017), examining 26 activity-based studies published after 2010, including specifics on parameters. (Miola & Ciuffo, 2011) also conduct a critical examination of the current emission modeling methodologies and data sources (including AIS data), highlighting their limits and constraints.

The EMEP/EEA inventory Guidebook (EMEP/EEA, 2019) is one of the key emission factor databases that are extensively utilized throughout Europe (Grigoriadis, et al., 2021). EMEP/EEA source class comprises all water-based transportation, from small recreational vessels to large ocean-going cargo ships, that is powered mostly by high, slow, and medium-speed diesel engines, with steam or gas turbines, including hovercraft and hydrofoils. The inventory covers emissions of CO_2, CH_4, N_2O, CO, non-methane volatile organic compounds (NMVOCs), SO_2, PM, and NOx.

Regarding the last IMO goal, in 2000, the organization published its first study (IMO, 2000) about the situation and forecasting of global carbon emissions. Ever since, the second (IMO, 2009a) and third (IMO, 2014) GHG studies were published, the last one gave a thorough examination of data quality challenges and uncertainties in both top-down and bottom-up techniques. Afterward, in line with the Roadmap at Marine Environment Protection Committee (MEPC) 74th session in 2019, the Fourth IMO

GHG Study (IMO, 2020) provides an inventory of GHG and air pollution emissions from shipping for the period between 2021 and 2018 and presents emissions projections for the period between 2018 and 2050. On the document, it is presented a methodology to estimate emissions from gases considered in the United Nations Framework Convention on Climate Change (UNFCCC); NOx; non-methane volatile organic compounds (NMVOCs); CO; PM and SO_X; and black carbon (BC), as partially implemented on the software used in this study and described in the Methodology section. A detailed discussion about the status and prospects of the decarbonization of maritime transport based on GHG IMO studies can be found in (Psaraftis & Kontovas, 2020).

Nevertheless, some remarks must be made about the limitation of AIS-based models as described in the last GHG IMO study. Firstly, (Psaraftis & Kontovas, 2020) highlight that weather influence imposes significant fuel consumption for the same instantaneous ship speed, which effect is approximated by an independent constant (sea margin). Further uncertainties can be mentioned in the data-driven methodology, such as design speed database accuracy (Psaraftis, 2019), speed over ground use instead of through water, and ship draft approximations.

In the maritime sector, emission factors are most expressed about energy output, i.e., the mass of pollutant per unit of energy produced by the engine (g/kWh), so-called energy-based emission factors EF_e, or per unit of fuel consumed (g/g), so-called fuel-based emission factors EF_f. In a limited number of studies, distance-based emission factors in g/nm are also presented (Grigoriadis, et al., 2021).

On the other hand, inland waterway transportation (IWT) has received less attention than maritime transportation, in terms of environmental damage assessment and regulations. Since more than 95% of inland ships are propelled by Diesel engines, with average motor age of 40 years (UBA, 2012), air exhaust pollutants are like ocean-going vessels and consequently, negative effects from freight transport along rivers and channels cannot be neglected.

To evaluate the impact on the environment caused by barges and convoys, a literature review took place using the *ScienceDirect* database, in which keywords for searching were “inland waterway emissions” between 2012 and 2022 publications. Among 1838 papers obtained, sorted by relevance, 11 papers were selected and followed presented. However, a more general taxonomy of sustainability issues for papers published between 2015 and 2020 is presented in (Barros, et al., 2022) and, focused on IWT in intermodal supply chains, by (Caris, et al., 2014).

The applicability of modern alternatives for inland ship power systems, such as lithium batteries and hybrid powered ships (LNG and battery modulus), and abatement technologies (mainly scrubber and green fuel) was the focus of several studies. For instance, (Fan, et al., 2021) evaluated environmental and economic impacts and uncertainty analysis method during the life cycle, demonstrating that battery-powered ships and hybrid-powered, compared to the traditional Diesel power scheme, have 14.5% lower CO_2 emissions and, considering fuel costs, the total cost is 17% lower. For achieving significant pollutant abatements with LNG-fueled barges, (Ursavas, et al., 2020) implemented heuristic models for supporting infrastructure development along the waterway network in the Arnhem-Nijmegen region in the West-European River network. Additionally, (Tan, at al., 2022) investigate both scrubber installation and green fuel utilization (MGO) based on cost minimization and its relationship with streamflow speed, showing that the scrubber option presents a solution with optimum speed higher than the MGO appliance.

Many other strategies for reducing air emissions are related to regulatory and operational strategies. (Xu, at al., 2021) has simulated by a tripartite evolutionary game model that environmental governance of inland navigation had to synergistically act with shippers to promote the electric ship industry for reducing the environmental pollution. Moreover, a speed optimization based on fuel consumption minimization within an inland waterway network can be responsible for assessing environmental and economic criteria. Regarding operational measures, (Golak, et al., 2022) implemented a heuristic algorithm for solving the lock scheduling problem of the Dutch river network, allowing lock operators and vessel skippers to determine sailing speed regarding fuel consumption and CO_2 emissions minimization.

Not only inland transportation negatively impacts the environment, as GHG emissions, but also the service level can be more affected by Climate Change than inland transport modes. As analyzed by (Christodoulou, et al., 2020), climate change is responsible for modifying river’s water levels, which implies reductions in vessel load or even navigability within channels. However, taking into consideration uncertainties related to the methods applied, the conclusion obtained is that inland waterway transport is one of the few sectors where climate change can have a negligible or even positive impact.

Besides inland waterways are mostly located in rural areas, ship exhaust emissions are especially concerning for densely populated areas where many inhabitants reside in direct proximity to rivers. (Keuken, et al., 2014) and (Zee, et al., 2012) have studied air pollutant levels in The Netherlands associated with vessel traffic close to residential areas. Both studies have considered actual downwind measurements of particle numbers and nitrogen oxides, and PM emission factors were derived in (van der Zee, et al., 2012) for the Rhine Canal. A comparative analysis of metal, polycyclic aromatic hydrocarbons (PAH), and PM emissions in inland navigation vessels, domestic heating, and ocean-going vessels were carried out by (Bläsing, at al., 2016) using experimentation of existing ships and house heating systems and literature values. It was shown that for most metals and particulates, OGVs presented higher emission levels than barges and convoys, especially considering the youngest inland vessels with particle filters.

2.2 Externalities in Transportation Sector

2.2.1 External costs components

Current fuel prices and new emission restrictions can significantly affect more sustainable transport segments if no additional measures are adopted, i.e., avoid shifts to land-based modes that face typically more pollutants than waterborne transportation (Zis, et al., 2019). In this sense, the concept of external costs can be applied to measure the intensity of negative impacts generated by different modes of transport, and when applied to the cost structure, the modal shift can be avoided in favor of modes less pollutant and harmful to human health.

In the transportation sector, (CE Delft, 2019) classifies external costs into nine categories: accidents, congestion, noise, air pollution, climate change, Well-to-Tank (WTT) emissions, habitat, and infrastructure. Each one of these parcels is related to a different externality caused by transport activity or its infrastructure. However, other classifications can be found in the literature, such as photochemical ozone formation, and specific particulate matter formation, as studied in (Merchan, et al., 2019) for inland freight transport modes in Belgium.

Air pollutant and climate change costs are costs related to externalities caused by exhaust gas emissions, and it is associated to all modes of transport. Air pollutant emissions are related to several human health problems but are also extended to material and biodiversity losses. Energy-related air pollutants, PM, and NO_X are largely associated with a higher risk of respiratory and cardiovascular diseases, leading to medical treatment costs, production loss at work, and even death (CE Delft, 2019). Additional issues addressed by air pollutants, such as NO_X, NH_3, and SO_X are crop damage, corrosion on buildings, acidification of soil, precipitation and water, and the eutrophication of ecosystems.

Another air pollutant from transportation is the greenhouse gases (GHG) emissions, as already mentioned, associated with environmental problems related to global warming. Freight transportation of heavy-duty cargoes is usually carried out by vehicle with internal combustion engines, often fueled by Diesel, depending on the transport mode. Problems associated with sea level rise, biodiversity loss, water management issues, frequent weather extremes, and crop failures are taken into consideration in this classification.

Also applicable in all modes of transport, the Well-To-Tank cost (WTT) takes into consideration up and downstream processes related to transport that led to negative external effects, such as emissions caused by energy production, but it is not related to direct harmful effects of vehicles emissions. Different than Tank-to-Wheel emissions (or Tank-To-Wake in maritime transport), processes of extraction of energy sources, processing (e.g., refining or electricity production), transport and transmission, the building of energy plants and other infrastructures lead to emission of air pollutants, greenhouse gases, and other substances, composing a relevant parcel of the total external cost (CE Delft, 2019).

As recently introduced on the software used in this thesis, the habit damage is additional negativity associated with the transportation sector. Among the consequences of air pollutant emissions and transport infrastructure, this category comprises ecosystem loss, habitat fragmentation, and habitat degradation. Natural habitats of plants and animals can suffer considerable reduction when transport infrastructure requires land surfaces, impacting not just during the building phase but also during the infrastructure lifetime. Large and broad main infrastructures such as motorways and high-speed rail lines also impose population discontinuities by imposing physical barriers.

There are only a few studies covering the external costs of habitat damage due to transport activities. (ECOPLAN; INFRAS, 2014) presents the external and social effects on the environment in Suisse in 2010, concerning also externalities related to habitat fragmentation and extinction, which cost computed could vary between -22% and 27%. External cost in EUR/v-km was obtained from Germany in (UBA, 2019), in which the rates were based on the costs for (virtually) restoring lost biotope or ecosystem areas and, in the case of habitat fragmentation, based on the costs for (virtually) constructing defragmentation structures. In the case of (CE Delft, 2019), the habitat damage cost is calculated based on the infrastructure network length or area, and then, based on the EU28 average values, cost factors for all countries have been calculated, in EUR/v-km.

Marginal cots assume different forms depending on the transport mode analyzed or, in some cases, they are not applicable due to lack of information or not significant compared to other external parcels. Table 2.1 presents external cost components as a function of different aspects (regulation, region, or vehicle characteristics) according to maritime, road, rail, and IWT modes of transportation.

2.2.2 Impact of internalization externalities on the SSS competitiveness

For now, the literature about negative effects of the transportation activity were discussed, comprising a bigger understanding of the different ways for classifying external costs in different modes of transportation. Independently of the form in which externalities are presented, the focus of international efforts for a sustainable development is how to make the polluters responsible for the consequences of their sector in way to reduce the overall emissions. However, many efforts for internalizing external costs have not succeeded in building legal measures (Profillidis, et al., 2014), among many reasons such as the difficulty of monetize externalities accurately.

The internalization of external costs is responsible for making the transport sector accountable for the full costs of his transport decision. It can be achieved, for instance, through carbon pricing and infrastructure charging (Santos & Ramalho, 2021b). On the literature, several authors have analyzed external cost internalization policies in different way, such as (Beuthe et al, 2002), (Macharis, et al., 2010), (Moliner, et al., 2013), (Agarwal, et al., 2015), (Austin, 2015) and (Dente & Tavasszy, 2018); and also for optimization objectives, as (Mostert, et al., 2018), (Musso & Rothengatter, 2013), (Santos, at al., 2015) and (Zhang, et al., 2015).

Currently center of attentions, the pricing for carbon emissions based on emission trading systems allows a carbon credit to be traded, i.e., allows the company that holds the right to emit a certain amount of carbon dioxide or other GHG to sell to another company. In accordance with the climate action plan proposed by the European Commission, the Emissions Trading System (EU-ETS) (EC, 2003) was created in 2005 as the world's first international emissions trading system, working with the mentioned cap-and-trade mechanism. By this mechanism, the quantity of emissions allowed (cap) that can be traded is reduced over time so that total emissions fall. The price traded in this system is the carbon permit can vary significantly according to the social and economic situation. For instance, EU ETS carbon credit recorded its highest values in 2022, with about 99EUR/ton of CO_2 due to combined factors of the current shortage of natural gas and consequent increased demand for coal, a pollutant energy source (Financial Times, 2022).

Table 2.1 – External costs dependence per transport mode

External Cost	Inland water Transport	Maritime Transport	Road transport	Rail transport
Air Pollution	- *Vessel Type:* CEMT II, Va or Convoy - *Emission class:* CCNR 0, 1 or 2 Link type: rural or urban	- *Ship type*: RoPax, container ship, or bulk vessel - *Size*: Small or Large - *Distance* *Tier*: 0, 1 or 2	- *Fuel*: Diesel or LNG - *Vehicle segment*: rigid or articulate and category *EURO* - *Standard*: EURO 0 to 6 - *Road area*: metropolitan, urban, or rural - *Road type*: motorway, urban, rural	- *Freight transport type*: short or long container - *Traction*: electricity or diesel - *Abat. Tech*.: with or w/o EGR/SRV - *Link type*: metropolitan, urban, or rural
Climate Change	- *Vessel Type*: CEMT II, Va or Convoy	- *Ship type*: RoPax, container ship or bulk vessel - *Size*: Small or Large - *Distance*	- *Fuel*: Diesel or LNG - *Vehicle segment*: rigid or articulate and category - *EURO Standard*: EURO 0 - 6 - *Road type*: motorway, urban, rural	- *Freight transport type*: short or long container Traction: diesel
Well-To-Tank	-*Vessel Type*: CEMT II, Va or Convoy	- *Ship type*: RoPax, container ship or bulk vessel - *Size*: Small or Large - *Distance*	- *Fuel*: Petrol, Diesel, or LNG *Vehicle segment*: rigid or articulate and category - *EURO Standard*: EURO 0 - 6 *Road area*: metropolitan - *Road type*: motorway, urban, rural	- *Train type*: passenger (highspeed, intercity, or regional) or freight (short or long container) - *Traction*: electricity or diesel
Accident	- *Link country*: EU countries	N/A	- *Link country*: EU countries - *Road type*: urban, motorway, or rural	- *Link country*: EU countries
Noise	N/A	N/A	- *Link type*: metropolitan, urban, and rural - *Time of the day*: day or night - *Traffic situation*: thin or dense	- *Link type*: metropolitan, urban, and rural - *Time of the day*: day or night - *Traffic situation*: thin or dense
Congestion	N/A	N/A	- *Link country*: 28 EU countries - *Zone*: suburban, urban, or rural - *Type*: Over Congested or Near	N/A
Habitat	- *Link country*: EU countries	*N/A*	- *Link country*: 28 EU countries	- *Link country*: 28 EU countries - *Traction*: electricity or diesel

Announced in December 2021, the EU is developing and implementing a new package of proposals so-called 'Fit for 55' focused on an ambitious target of reducing net emissions by at least 55% by 2030 compared to 1990 and for being the first climate neutral continent by 2050. Among other scopes of action, the strategy adopted is to extend EU-ETS to maritime, road transport, and buildings over the period 2023 to 2025 (EC, 2022). As studied by (Christodoulou, et al., 2021), the extension to cover CO_2 emissions from the maritime sector has a strong negative impact on the competitiveness of Ro-Ro and Ro-Pax segments against other modes of transportation, encouraging modal shift from sea to land-based modes whether ship operators do not invest in energy-efficient technical and operational measures and alternative or renewable fuels. The emission allowance fee is a way of internalizing the negative externalities from shipping and considerable funds that are generated from the EU ETS provide capital for environmental projects (Cariou, et al., 2021), even with low carbon prices.

A carbon leakage can also be a side effect of the introduction of the maritime sector in the EU EST system in the context of Fit for 55 packages. When a business decides to shift its activity from a nation with strict regulation to one with laxer ones, it causes a rise in GHG emissions, known as carbon leakage. The EU Emission Trading System has negative implication to container vessel lines in the European Economic Area (EEA) (Lagouvardou & Psaraftis, 2022). Considering only cost criteria, international services may relocate to ports outside EEA motivated by reduction on the savings with EU Allowances, leading to carbon leakage and revenue loss for the EU ETS. Therefore, even if maritime transport is still a viable option for shippers, the abatement of emissions is not attained whether measures do not cover an extensive scope of action, and negative economic impact may be an additional consequence.

Emission trading systems is an example of Market-based Measure (MBM) centered on the idea of external cost internalization by means of polluter pays principle. The purpose of such measures is to induce operational and technical adaptations aiming to reduce air pollutant emissions. In the maritime transportation sector, the preferable behavior changes are the speed reduction in short run and option for alternative fuels and stimulation for the use of abatement technologies in long run (Psaraftis, at al., 2021). Among 11 measures discussed on the context of international IMO measures in 2010, another important MBM is a bunker levy may provide considerable GHG reductions depending on the levy intensity, but legal obstacles since is not compatible with existing legal frameworks.

(Mostert & Limbourg, 2016) identifies recent work achieved in the field of external costs of road and intermodal freight transport, covering objective, type of externalities, and the type of cost (marginal, average, total) considered in the literature. The impact of transport costs and air pollution external costs is analyzed by (Mostert, et al., 2017) for road and intermodal transport in Belgium, regardless of maritime transportation. Results showed an increasing share of intermodal transport by external cost minimization since rail and IWT modes are less harmful to the environment than road mode. Using an economic optimization strategy by incurring road taxes, the road market share compared to the intermodal transport share decreases, but it leads to an underuse of intermodal transport, compared to the environmental optimization strategy.

(Vierth & Merkel, 2022) exposes the case of Sweden regulatory system for internalizing external costs in ships, aiming to compare it to real societal costs generated by the segment. The national internalizing system consist of fairway dues based on environmental ship performance on CO_2, NO_X, SO_X, and PM emissions, going into a different direction of current regulation that aims to penalize maritime transport to reduce emissions. The paper computes marginal and infrastructure costs using AIS statistics to compute ship's emission with a bottom-up approach. The degree of internalization achieved depends on the method for computing external costs and from the ship segments analyzed, ranging from 53% to 90% of external costs. On the other hand, the internalization covers a small parcel of cost when considered new developments of Swedish guidelines.

The objective of (Santos G. , 2017) study comprises the evaluation of the percentage of external cost internalization in the current taxation policies in road transportation in Europe. The degree of internalization again is based on the comparison between the computed external costs to society and fuel taxation and efficiency. It was concluded that Diesel taxation is not enough for balance externalities from commercial vehicles in most of the 22 EU countries analyzed by the paper, given space for further evolutions on HDV taxation based on environmental performance. In this segment, the best performance taxes over the fuel price are between 40% to 45% of the corrective taxation intended to cover all external costs in Spain, Portugal, and Italy. An important behavior that must be noticed is the difficulty of taxation policy regarding that HDV refuel in countries where Diesel is cheaper, and a policy must consider this aspect in order to produce significant abatements.

To evaluate the environmental competitiveness of SSS and road-only transportation (Vallejo-Pinto, et al., 2019) established a methodology based on map visualizations of so-called iso-emissions maps, presenting geographical regions that can be connected by SSS and road with the same level of emissions. The geographical scope of more environmentally friendly modes is determined by GHG emissions rather than the monetization of its negative impacts. The case study considers transportation from different origin points to the port of Gijón (Spain) and then by sea to the port of Saint-Nazaire (France), finally heading to several destinations in France. Results show that some important French regions are reached with fewer air emissions by shifting from road mode to the SSS, and the higher the load factor of the ship, the wider the geographical scope for which SSS is preferable.

(Santos & Ramalho, 2021a) have studied in detail the numerical methods applied in a decision-making tool for computing emissions in intermodal transport chains. Additionally, results are shown to routes connecting Portugal to central Europe, in which the maritime mode is conducted by vessels with the same capacity and installed power but fueled by VLSFO and equipped with scrubber and Selective Catalytic Reduction, or simply fueled by LNG. The results demonstrated a significant reduction in air pollutant emissions by adopting LNG fuel, but the economic aspects of power system installation cost and fuel purchase cost were not considered. Furthermore, the numerical tool was expanded to compute external costs according to (CE Delft, 2019) for the same geographical scope in (Santos & Ramalho, 2021b) and the best route could be determined by external cost internalization for a set of destination connected by different routes, demonstrating the importance of more intense externalities monetarization to reduce transport externalities.

3. METHODOLOGY

This section presents the numerical procedure to compute air pollutant emissions and the methodology for computing external costs associated with transportation. In each mode of transport, the energy and fuel consumption are computed using a bottom-up approach, and then the air pollutant emissions are calculated using emission factors. For doing this, the power demand estimation and the specific fuel consumptions are presented, considering vehicle' specific characteristics and abatement technology, when applicable. To conclude, the methodology to compute the total external costs and their parcels through marginal costs is described.

3.1 Method for Calculating Emissions

The methodology for computing PM, $CO_{2\text{-eq}}$, NO_X, and SO_2 emissions is divided into the fuel-based method, in which emission factors directly relate the mass of pollutant emitted to the mass of fuel consumed [g/g], or energy-based methods, in which emission factors relate the mass of pollutant to the energy required [g/kWh] (IMO, 2020). The formulations for computing emissions applying both factor categories are similar, in the first case it is just required an additional step for computing the fuel consumption. Therefore, the basic procedure for all transport modes is to estimate the power based on specific vehicle technical characteristics, then the fuel consumption is computed, and applying emission factors, the air pollutant emissions are finally obtained.

3.1.1 Road transportation

The truck's fuel consumption, in mass, may be estimated by multiplying the specific fuel consumption (in g/kWh), the power demand (in kW), and the time spent on the link (in hours). The specific fuel consumption is an input on the software, allowing easy variation regarding truck type, the power estimation is based in basic physical laws, also using vehicle' specification, and the time may be computed through speed and distance data.

A tractive power demand estimation follows an approach of energy required to balance truck's forward acceleration and resistance forces that oppose to the movement of the truck. The truck resistance forces in link k, part of path j (part of the transport chain that connects the origin to destination i), are divided into inertial force F_I due to trucks acceleration, rolling force F_r due to friction between the tires and asphalt, drag force F_d due to air resistance, and grade force due to road gradient F_g:

$$F_{I,ijk} = M_{ij} \cdot \frac{dV_{ijk}}{dt} \tag{1}$$

(2)

$$F_{d,ijk} = \frac{1}{2} \cdot \rho_{air} \cdot C_d \cdot A_f \cdot \left(\frac{V_{ijk}}{3.6}\right)^2 \tag{3}$$

$$F_{r,ij} = C_{rr} \cdot M_{ij} \cdot g \cdot \cos\theta \tag{4}$$

$$F_{g,ij} = M_{ij} \cdot g \cdot \sin\theta \tag{5}$$

in which ρ_{air} is the air density (in kg/m^3); g is the acceleration of gravity (in m^2/s); C_d is the drag coefficient; A_f is the frontal area (in m^2); C_{rr} is rolling resistance coefficient; θ is the road gradient (in rad); V_{ijk} is the link speed (in km/h); and M_{ij} is the truck gross weight (in kg), including cargo and tare weights.

The transport network covers a great extension of roads in Europe and some simplifications were made to limit the scope of the thesis to emission computations, avoiding details about road topology and specific data track. Then, some assumptions were made:

- Truck is travelling at constant speed. Consequently, truck acceleration (dV_{ijk}/dt) is considered null and the inertia force is disregarded.
- The road is considered plane. The road gradient (θ) is then null, and the force required to truck overcome inclined roads is zero ($\sin\theta = 0$).

The total resistance force $F_{T,ijk}$ simplified and applied on the software calculation is basically given by the equation:

$$F_{T,ijk} = \frac{1}{2} \cdot \rho_{air} \cdot C_d \cdot A_f \cdot \left(\frac{V_{ijk}}{3.6}\right)^2 + C_{rr} \cdot M_{ij} \cdot g \tag{6}$$

To account mechanical losses in transmission, the power demand $P_{D,ijk}$, in kW, is function of the transmission efficiency η_t, given as:

$$P_{D,ijk} = \frac{F_{T,ijk}}{\eta_t} \cdot \frac{V_{ijk}}{3.6} \tag{7}$$

All parameters necessary to compute the power demand on road transport mode were extracted from the base case in (Gao, et al., 2015) and the summary can be seen in Table 3.1 below.

Table 3.1 – Road power parameters

Parameter	**Variable**	**Value**	**Unit**
Air density	ρ_{air}	1.225	[kg/m^3]
Gravity	g	9.81	[m^2/s]
Rolling resist.	C_{rr}	0.007	[-]
Drag coefficient	C_d	0.58	[-]
Frontal area	A_f	10.38	[m^2]
Transmission efficiency	η_t	0.85	[-]

Congestion is a relevant phenomenon to be taken into consideration for computing truck's emissions since some stretches of road experience traffic that increasing travelling time and consequently, harmful driver exposure to air pollutants. The approach adopted considers in applying speed reduction coefficients to database average road speeds in Equations (6) and (7).

The road volume corresponds to the number of vehicles that crosses a certain road point over a certain period and capacity is the maximum number of vehicles in a road stretch. In Traffic Flow Theory, the ratio between these two parameters determines the congestion condition and using the curve speed-flow, the speed reduction may be obtained. In the database, each link is characterized by a congestion level, previously determined by volume-capacity ratio, and Table 3.2 (CE Delft, 2019) presents the speed reduction coefficient applied to each link speed depending on its congestion level.

Table 3.2 – Congestion level and speed reduction in road mode

Congestion level	Volume/Capacity ratio (V/C)	Speed reduction
1	$V/C < 0.4$	V_{ijk}
2	$0.4 \leq V/C < 0.8$	V_{ijk}
3	$0.8 \leq V/C < 1$	$0.75 \cdot V_{ijk}$
4	$1 \leq V/C < 1.2$	$0.5 \cdot V_{ijk}$
5	$V/C \geq 1.2$	$0.4 \cdot V_{ijk}$

Generally, p air pollutant emission, based on energy methods, are computed directly from the energy-based emission factor $EF_{e,p}$, in g/kWh, multiplied by the power demand, in kW, and time on the link, in hours, given by the link distance L_{ijk} divided by link speed V_{ijk}. Then, for PM and NO_X emissions are given by:

$$E_{ijk,p} = EF_{e,p} \cdot P_D \cdot \frac{L_{ijk}}{V_{ijk}} \tag{8}$$

On the other hand, the fuel-based method applies factors in g/g and the fuel consumption can be obtained by the power, in kW, multiplied by the specific fuel consumption, in g/kWh, and time on the link, in hours. Then, $CO_{2\text{-eq}}$ and SO_2 emissions are given as:

$$E_{ijk,p} = EF_{f,p} \cdot SCF_{ij} \cdot P_D \cdot \frac{L_{ijk}}{V_{ijk}} \tag{9}$$

The fuel consumption of trucks is usually given as mass (or volume) of fuel consumed per kilometer of travelled distance, however the approach here considers the fuel consumption per unit of time and energy demand. Even though both approaches are interchangeable, the chosen methodology facilitates the use of manufacturer data. Considering a heavy-duty truck applied in long-haul transport in Europe, the specific Diesel fuel consumption was assumed to be 215 g/kWh (FVT, 2018; COST, 2005). Such parameter is representative of several steady-state tests of engine for truck's EURO standard classification. The degradation of fuel-efficiency over lifetime was disregarded in this study.

For road transport mode, emission factors were considered to follow the current regulation in the European Union, when applicable. For energy-based air pollutants, NOx and PM limits are determined by European standards for heavy-duty Diesel engines used in trucks, presented by Directives 88/77/EEC, 05/55/EC, 2001/27/EC, 2005/55/EC, and regulation 595/2009.

According to (Olmer, et al., 2017), the SO_2 emission factor, in g/g, is computed by the equation below as a function of the sulphur content present SC, in ppm, on the fuel in analysis.

$$EF_{f,SO_2} = 2 \cdot 0.97753 \cdot SC \cdot 10^{-6} \tag{10}$$

Automotive Diesel fuel quality in Europe is specified by the EN 590 standards since 1993. For all Member States, the Euro V standard has established a maximum permissible sulphur content of 10 ppm after 2011 for road and non-road (including inland waterways vessels) mobile machinery (EU, 2009). For LNG-fueled trucks, the sulphur content was assumed to be 4 ppm. Table 3.3 summarizes the emission factors established by EU regulations regarding emission standard and sulphur fuel quality as mentioned above.

Table 3.3 – NO_X and PM emission factors and sulphur content for heavy-duty Diesel engines

EURO standard	**NO_X [g/kWh]**	**PM [g/kWh]**	**SO_X [ppm]**
1	8	0.36	2000
2	7	0.15	500
3	5	0.1	350
4	3.5	0.02	50
5	2	0.02	10
6	0.4	0.01	10

The emission factor from the mass of fuel to the mass of $CO_{2\text{-eq}}$ emitted considers the most relevant pollutants responsible for global warming, carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O). Thus, the equivalent emission factor is the sum of each pollutant factor weighted by their global warming potential, resulting in 3.181 g/g for Diesel engines and 3.104 g/g for LNG engines.

3.1.2 Rail transportation

The basic procedure for computing road transport emissions is applied to the rail transport. Firstly, the power and fuel consumption are estimated and then, the air pollutant emissions are obtained through emission factors. However, a new concept is introduced to compute the locomotive power demand in trains and the fuel consumption is directly given by mass of fuel per kilometer.

Emissions in rail transport are computed for a line-haul locomotive propulsion unit, electric or Diesel, used in long-distance container freight contained transport in Europe. The locomotive power calculation applies the energy consumption data provided by (CE Delft, 2021), in which energy coefficients are given in power demand per train gross-tonnage weight (GTW) per kilometer displaced (MJ/tkm). The energy coefficients were computed based on measurements of emission and energy consumption data extracted from several reports from the Dutch railway manager ProRail.

In container transport, train categories are defined by the cargo load carried (light, medium-weight, and heavy transport) and by the train length (long and extra-long). Therefore, defined the weight of the cargo unit (cargo load) and chosen the train length category, the gross-tonnage weight, i.e., the sum of cargo weight and empty wagons weight, can be approximated. Table 3.4 provides information used to classify the train by length and load, and based on these two classes, the GTW of the train in analysis.

Table 3.4 – Train category definitions

Load category	Length category	Length [m]	Load capacity [FEU]	GTW [t]
Light transport (12 ton/FEU)	Long	635	44	988
	Extra-long	719	50	1,123
Medium-weight transport (21 ton/FEU)	Long	626	45	1,270
	Extra-long	727	52	1,481
Heavy transport (28 ton/FEU)	Long	650	48	1,595
	Extra-long	729	54	1,795

The power demand $P_{D,ijk}$, in kW, is given by multiplying the energy consumption EC_{ij}, in MJ/tkm, to the train gross-tonnage weight $GTW,$ in ton, and specific link speed, in km/h, as shown in the equation below.

$$P_{D,ijk} = \frac{EC_{ij}}{3.6} \cdot \ GTW \cdot V_{ijk} \tag{11}$$

in which 3.6 is the energy conversion from MJ/tkm to kWh/tkm.

Table 3.5 presents the energy coefficients per cargo load and length classification, and locomotive type (electric and Diesel). This methodology provides a more accurate estimation of emissions than considering a fix installed power, allowing the determination of load power usage based on different operational profiles according to the train speed. Additionally, a differentiation of railway transportation based on the train locomotive types and length allows the characterization of very different emission scenarios that can be found in different parts of the European continent. The accuracy of such approach is considered suitable considering that the secondary source provided real EU data in important railway conditions.

Table 3.5 – Energy consumption coefficient per train length and load class and locomotive type

Load	Locomotive type	Train Length	EC [MJ/tkm]
Medium load	Electric	Long	0.11
		Extra-long	0.10
	Diesel	Long	0.29
		Extra-long	0.27
Light load	Electric	Long	0.18
		Extra-long	0.16
	Diesel	Long	0.48
		Extra-long	0.44
Heavy load	Electric	Long	0.08
		Extra-long	0.07
	Diesel	Long	0.22
		Extra-long	0.20

Energy-based pollutant, PM and NO_X are then computed by applying proper emission factors and link characteristics in Equation (8). Like the road transport mode, energy emission factors are also regulated by the European Commission by setting emission limits. The emission factors, in g/kWh, adopted in this study are defined by Directive 2010/26/EU and Regulation 2016/1628, regarding non-road mobile machinery standards Stages III and V, respectively. The PM and NO_X factors are applied to 130 kW Diesel engines and above and it is function of the locomotive net power and category – railroad and railcars locomotives – according to Stage III, and the Stage IV is applicable to rail locomotives and railcars without power restriction. Since this thesis covers container freight transport, only locomotives are considered as mean of train traction. Table 3.6 presents NO_X and PM emission facts extracted from the current engine standard directives per train category.

Table 3.6 –NO_X and PM emission factors for rail Diesel engines traction

Stage	Category	NO_X [g/kWh]	PM [g/kWh]
III-A	Railcar	4*	0.200
	Locomotive (RL)	4*	0.200
	Locomotive (RH)	6	0.200
	Locomotive (RH)**	7.4	0.200
III-B	Railcar	2	0.025
	Locomotive (R)	4*	0.025
V	Locomotives	4	0.025
	Railcar	2	0.015

*Considers HC emission. **for locomotives above 2,000 kW

For computing the fuel consumption, a typical Diesel engine fuel consumption of FC_{ij} = 219 kg/hour (EMEP/EEA, 2019) was assumed, and then pollutant p emission is given by the emission factor $EF_{f,p}$, in grams of pollutant per gram of fuel burned and link characteristics.

$$E_{p,ijk} = 1000 \cdot EF_{f,p} \cdot FC_{ij} \cdot \frac{L_{ijk}}{V_{ijk}} \tag{12}$$

Adopting a conventional fuel oil sulfur content of 10 ppm, the same Diesel fuel quality requirement established to HDV, the SO_X emission factor was obtained by applying Equation 10. For the last fuel-based emission, $CO_{2\text{-eq}}$ factors were computed by summing the emission factors of main GHG pollutants and weighting them by the global warming potential, resulting in 3.1515 g/g for Diesel locomotives.

Emissions abatement technologies available for Diesel railway engines can be adopted on the software. The use of Diesel Particulate Filter (DPF) provides significant reduction in particulate matter emission factor and Exhaust Gas Recirculation (EGR) represents cuts on nitrous oxides, as presented in the Table 3.7 (EMEP/EEA, 2019). Whether the Diesel locomotive comprises with the Stage V standards for PM emissions, it is already assumed that the trains is equipped with DPF technology (EPA, 2018). For railways, it was considered that 95% of calculated PM_{10} is $PM_{2.5}$.

Table 3.7 – Emission abatement in technologies available for Diesel locomotives

Air pollutant	DPF	EGR/SCR
NO_X	-	-50%
PM	-99%	-

Electric locomotives may also be analyzed by the software. In this case, air pollution emissions are not considered since the methodology here presented covers only Tank-to-Wheel (TTW) emissions, only related to exhaust emissions resulting from combustion. Even though Well-to-Tank (WTT) emissions are not estimated in mass, its negative effects to human health and environment are considered in form of external costs, as will be presented in subsection 3.2.

3.1.3 Maritime transport

The fuel consumption on the waterborne transport is basically carried out by the main and auxiliary engines, responsible for the ship's propulsion and electric generation onboard, and shaft generators. The power demand varies according to the vessel's operational phases, classified according to its main engine power load:

- Cruise phase: occurs when the vessel is navigating at sea with its main engine load above 25%.
- Maneuvering phase: identified when the vessel enters or exits coastal waters and proceeds towards or departs from a berth or jetty and it is characterized by the main engine load below 25%.
- Port phase: the vessel is simply anchored at the destination node located in an existing port.

The main engine fuel consumption $FC_{ME,ij}$ on the maritime transport path j, part of the pair origin-destination i, is the sum of the fuel consumption in cruise profile (at sea) $FC_{ME,ij}^{sea}$ and maneuver profile $FC_{ME,ij}^{mano}$:

$$FC_{ME,ij} = FC_{ME,ij}^{sea} + FC_{ME,ij}^{mano} \tag{13}$$

For each component, the fuel consumption is determined by the power demand and technical characteristics of the machinery. For the vessel's main engine, the fuel consumption $FC_{ME,ij}^{sea}$ on the maritime path j can be calculated knowing the power consumption, composed by the effective power $P_{EF,ijk}$ for propulsion, in kW, summed to the shaft generators power PTO_{ij}, in kW, with a load utilization factor of L_{PTO}^{sea}. Applying the specific fuel consumption of the main engine $SFC_{ME,ijk}$, in g/kWh, the vessel's speed in the link V_{ijk}, in km/h, and the link's length L_{ijk}, in km:

$$FC_{ME,ij}^{sea} = \sum_{k=1}^{K} SFC_{ME,ijk} \cdot (P_{EF,ijk} + L_{PTO}^{sea} \cdot PTO_{ij}) \cdot \frac{L_{ijk}}{V_{ijk}} \tag{14}$$

in which K is the number of links that compose the maritime path j part of the pair origin-destination i.

As will be shortly shown, the effective power demand $P_{EF,ijk}$ can be adjusted according to the vessel's speed and draught in each link k, accounting for the effect of link-related speed and different load capacity utilization. Firstly, the draft of the ship D_k is approximated by the variation of deadweight due to the change in number of cargo units.

Assuming a constant weight of each cargo unit W_{FEU}, the variation of deadweight at each link $\delta\varDelta_{ij}$ is:

$$\delta\Delta_{ij} = DWT_{ij} - W_{FEU} \cdot Cap_{ij} \cdot Ut_{ij} \tag{15}$$

in which DWT_{ij} is the vessel's design deadweight (in tons), Cap_{ij} is the vessel's capacity (in FEUs) and Ut_{ij} is cargo utilization factor. In the same way, the draught variation $\delta\varDelta_{ij}$ can be obtained from the change in displacement as:

$$\delta\Delta_{ij} = A_w \cdot \delta D_{ij} \cdot \gamma \Rightarrow \delta D_{ij} = \frac{\delta\varDelta_{ij}}{A_w \cdot \gamma} \tag{16}$$

Considering that the ship' sides of the vessel are parallel, the water plane area can be considered constant and then, the waterline length L_f and breadth B_f at initial draught can be estimated by the ship length between perpendiculars $L_{PP_{ij}}$ and moulded breadth B_{ij}, respectively. Using the water plane area coefficient c_w definition, here assumed as 0.671 for Ro-Ro ships, the water plane area A_w can be obtained by:

$$c_w = \frac{A_w}{L_f \cdot B_f} \Rightarrow A_w = c_w \cdot L_{PP_{ij}} \cdot B_{ij} \tag{17}$$

Applying Equations (13) and (14) in Equation (12), the draft variation can be obtained and the new corresponding draft D'_{ij} is:

$$D'_{ij} = D_{ij} - \delta D_{ij} = D_{ij} - \frac{DWT_{ij} - W_{FEU} \cdot Cap_{ij} \cdot Ut_{ij}}{c_w \cdot L_{PP_{ij}} \cdot B_{ij} \cdot \gamma} \tag{18}$$

Determined the draft of the ship under the new cargo condition, the effective output $P_{EF,ijk}$ now can be calculated at a given link speed V_{ijk}, in km/h, and for draught D'_{ij}, in m, can be estimated by.

$$P_{EF,ijk} = \frac{PME_{ij} \cdot \left(\frac{V_{ijk}}{V_{ij} \cdot 1.852}\right)^3 \cdot \left(\frac{D'_{ij}}{D_{ij}}\right)^{0.66}}{\eta_w \cdot \eta_f} \tag{19}$$

in which PME_{ij} is the installed main engine power and V_{ij} is the ship design speed, in knots, at 100% of maximum continuous rating (MCR) with clean hull and calm sea.

The formulation for the effective power corresponds to a variation of the Admiralty formula presented by IMO. In this case, the power demand is considered to have a cubic dependency with the speed ratio and a ship's displacement dependency powered by 1/3, which is translated to the ratio between drafts. Additionally, rough sea conditions and increasing hull surface roughness are responsible for increasing the fuel consumption to keep the same speed as a clean hull in a steady sea. These two effects – weather and fouling –, are considered by constant efficiencies $\eta_w$and η_f responsible for increasing the power demand. For Ro-Ro of more than 5000 DWT, η_w is 0.867 and for all ship types and sizes, η_f is assumed to be 0.917, according to IMO GHG 2020 report (IMO, 2020).

Even though the formulation has advantages regarding usability and is a cost-efficient method for estimating power demand, some remarks must be considered. The speed-power exponent is significantly lower than 3 at speed intervals below the design speed (Berthelsen & Nielsenac, 2021) and then speed reductions must be carefully adopted. The weather and fouling efficiency are constant values, but it has a strong influence in the region where the vessels sails and vessels age. The accuracy of the data used on the formula parameters is the focus of many uncertainties, such as speed over ground can be modified by existence of marine currents.

The last term to be defined to compute the fuel consumption at navigation profile is the specific fuel consumption $SFC_{ME,ijk}$, given as a parabolic variation with the percentage of utilization of the main engine, i.e., the main engine load $L^{sea}_{ME,ijk}$:

$$SFC_{ME,ijk} = SFC_{base} \cdot (0.455 \cdot {L^{sea}_{ME,ijk}}^2 - 0.710 \cdot L^{sea}_{ME,ijk} + 1.280) \tag{20}$$

in which:

$$L_{ME,ijk}^{sea} = \frac{P_{EF,ijk} + L_{PTO}^{sea} \cdot PTO_{ij}}{PME_{ij}} \quad (21)$$

The base specific fuel consumption is then an important parameter for the determination of the fuel consumption in certain main engine load condition. This parameter is provided by the engines manufacturer from curves obtained from engine tests, in which the lowest point of the curve represents SFC_{base}, the most fuel-efficient point that usually occurs at engine load around 80% MCR. The base specific fuel consumption SFC_{base}, expressed in g/kWh, is given to different engine rate speed (slow, medium and high speed) and fuel types (HFO, LNG, MDO, Methanol) at the most fuel-efficient point (around 80% MCR), according to IMO GHG 2020. All engines are considered third-generation engines build after the year 2000. It was assumed that SFC_{base} for residual low-sulfur fuels (LSHFO, VLSFO, and ULSFO) are the same as for HFO, as data is presented in Table 3.8 (IMO, 2020).

Table 3.8 – Basic specific fuel consumption for main engine

Rating speed	Fuel type	Basic specific fuel consumption [g/kWh]
Slow speed	HFO	175
	MDO	165
	Methanol	350
	LNG	148
Medium speed	HFO	185
	MDO	175
	Methanol	370
	LNG	156
High speed	HFO	195
	MDO	185

In some cases, estimated main engine load factor can be greater than 100% due to statistical deviations on the formulation (IMO, 2020). In order to avoid this statistical error, the link speed V_{ijk} is replaced by the design speed V_{ij} on the computation of effective output $P_{EF,ijk}$.However, after applying the hull, weather, draught, and speed-power adjustment factors, if the main engine load factor is still above 100% MCR, then the bottom-up model assigns a load factor of 98% MCR.

When the main engine load given by Equation (21) is below 25%, the vessel is assumed to be in the maneuvering profile, and in that case, just auxiliary engine power and shaft generator are operating. Shaft generators operate by means of burning fuel in the main engine at any given speed and loading condition, the fuel consumption in this operational condition uses the specific fuel consumption of the main engine. Usually, this parcel of power consumption is considered not significant compared to other power produced onboard (Smith, et al., 2016). However, in ships with considerable installed PTO, emissions can be underestimated by ignoring this parcel.

For the links identified with the maneuvering profile, a constant power load L_{AE}^{mano} is applied to the total PTO installed power, as given by the literature, or provided by the ship technical specifications. The main engine total fuel consumption in maneuvering profile is:

$$FC_{ME,ij}^{mano} = \sum_{k=1}^{K} SFC_{ME,ijk} \cdot (L_{PTO}^{mano} \cdot PTO_{ij}) \cdot \frac{L_{ijk}}{V_{ijk}} \tag{22}$$

For the fuel consumption of the auxiliary engine, a load usage percentage L_{AE}^{sea} and L_{AE}^{mano} of the total auxiliary engine power PAE_{ij} is used for computing fuel consumption $FC_{AE,ij}^{sea}$ and $FC_{AE,ij}^{mano}$ at sea and maneuvering operations, respectively. For emissions at port $FC_{AE,ij}^{port}$, fuel is assumed to be used along the number of hours spent moored $T_{P,ij}$ at an auxiliary engine load of L_{AE}^{port} of MCR. Thus, the total auxiliary engine fuel consumption is given as:

$$FC_{AE,ij} = FC_{AE,ij}^{port} + FC_{AE,ij}^{mano} + FC_{AE,ij}^{sea} \tag{23}$$

in which fuel consumption in each operational profile is:

$$FC_{AE,ij}^{sea} = \sum_{k=1}^{K} SFC_{AE} \cdot L_{AE}^{sea} \cdot PAE_{ij} \cdot \frac{L_{ijk}}{V_{ijk}} \tag{24}$$

$$FC_{AE,ij}^{mano} = \sum_{k=1}^{K} SFC_{AE} \cdot L_{AE}^{mano} \cdot PAE_{ij} \cdot \frac{L_{ijk}}{V_{ijk}} \tag{25}$$

$$FC_{AE,ij}^{port} = SFC_{AE} \cdot L_{AE}^{port} \cdot PAE_{ij} \cdot T_{P,ij} \tag{26}$$

Once the power demand and fuel consumption are determined, exhaust emissions are obtained using methods based on energy, in NO_X and PM emissions, or fuel emissions factors, for $CO_{2\text{-eq}}$ and SO_2 emissions. It is also assumed that low sulfur fuels have the same carbon emission factors as HFO. Regarding SO_X emissions, the fuel-based factors can be expressed as a function of the sulfur content in each type of fuel by Equation (10), in which 98% of the fuel sulfur is converted to SO_2. Table 3.9 presents the sulphur content, in percentage, and the correspondent emission factor per fuel type.

Table 3.9 – Sulphur content and SO_X emissions factor in marine fuel

Fuel Type	Sulphur content [%]	Emission factor [g/g]
HFO	2,6	0,0508
MDO	0,07	0,00140
LNG	0	0,0000317
MeOH	0	0,00264
LSHFO	1	0,0196
VLSFO	0,5	0,00978
ULSFO	0,1	0,00196
EN590	0,001	0,0000196

The mass of GHG emissions is computed by multiplying the fuel consumption previously described and the fuel-based $CO_{2\text{-eq}}$ emission factor, which directly relates mass of fuel burned to mass of GHG emissions. For computing the emission factor, emission factors of each GHG given by the Fourth IMO GHG Study is weighted by its global warming potential. Table 3.10 presents the resulting GHG emission factors in each fuel type. It was assumed that low sulphur fuels (ULSFO and VLSFO) have the same emission factor as HFO.

Table 3.10 – $CO_{2\text{-eq}}$ emission factors per marine fuel type

Fuel type	**$CO_{2\text{-eq}}$ emission factor [g/g]**
HFO	3.163
MDO	3.225
LNG	3.116
Methanol	1.375

Energy-based emission factors for PM and NO_X are a function of the engine load. As described in (IMO, 2020), a lower combustion efficiency is noticed when the main engine operated in low load. To represent such an effect, magnifying coefficients for increasing emission factors are introduced in the software when loading condition is above 10% MCR, and an increasing emission factor for load below 2% of installed main engine power.

On the case of particulate matter, emissions are composed by $PM_{2.5}$ and PM_{10}. As typically assumed on the literature, the total emission is obtained by computing PM_{10} and assuming that 92% of the calculated value is $PM_{2.5}$ (IMO, 2020). The computed PM_{10} emission factor is a function of the fuel's sulfur content, as presented by Table 3.9, and it is given for HFO and MDO/MGO, respectively, as:

$$EF_{e,PM_{10}} = 1.35 + SFC_{ij} \cdot 7 \cdot 0.02247 \cdot (S - 0.0246) \quad (27)$$

$$EF_{e,PM_{10}} = 0.23 + SFC_{ij} \cdot 7 \cdot 0.02247 \cdot (S - 0.0024) \quad (28)$$

in which S is the fuel sulfur fraction.

For LSHFO, VLSFO and ULSFO, the emission factor is given by Equation (20) with different sulfur contents. For pure LNG and auxiliary engines, the emission factor is assumed to be 0.02 g/kWh for LNG-Otto medium and slow speed and 0.01 for LNG-Diesel.

For computing NO_X emissions, the Tier emission limits are used as emission factors, depending also on the engine rated speed. In this study, medium speed engines are considered to have a rated speed of 500 rpm for applying the emission factor formulation which depends on the rating speed. For LNG-Otto medium and slow speed were assumed to have 1.3 g/kWh emission factor. Table 3.11 shows the NO_X emission factors per engine tier, depending on the engine speed rate category, as extracted from the fourth GHG IMO Study.

Table 3.11 - NO_X emission factor for marine engines with different tier and rating speed

Tier	NO_X emission factor [g/kW]		
	Slow speed	**Medium speed**	**High speed**
I	17.0	13.0	9.80
II	14.4	10.5	7.70
III	3.40	2.60	2.00

To convert NO_X and PM energy emission factors, generically represented by EF_e, to fuel-based factors, EF_f, the SFC_{base} may be applied as:

$$EF_f \left[\frac{g}{g}\right] = \frac{EF_e \; [g/kWh]}{SFC_{base} \; [g/kWh]} \tag{29}$$

The mass of emissions per pollutant p at maritime path j, connecting an origin/destination set i, also considering the emissions at port, is obtained by multiplying the fuel consumption by the emission factors, in g/g, in each machine:

$$E_{ijk,p} = FC_{ME,ij} \cdot EF_{p,ME} + FC_{AE,ij} \cdot EF_{p,AE} \tag{30}$$

Additionally, the numerical model can simulate the impact of abatement technologies by using a negative (reduction) or positive (increment) percentage of each pollutant emission, but also such equipment may be responsible for an additional fuel consumption. For instance, Wet Scrubber (WS) and Selective Catalyst Reduction (SCR) are responsible for reducing emissions in -80%, -97%, and -60%, for NO_X, SO_X, and PM emissions, respectively, and 2% fuel consumption increment. Another alternative for slow speed engines is the appliance of Wet Scrubber (WS) with Exhaust Gas Recirculation (EGR), responsible for decreasing -80%, -95%, -58%, for NO_X, SO_2 and PM emissions, but $CO_{2\text{-eq}}$ emissions and fuel consumption are incremented by 2% and 7%, respectively.

The same power and fuel consumption estimation methodology is applied to inland waterway transport (IWT), but some simplifications are assumed. Firstly, the power demand for propelling a self-propelled barge or pusher in a convoy is given by the original Admiralty formula, disregarding draught variation. Since auxiliary machinery onboard inland vessels are high speed generators with small installed power and usually moved by MDO/MGO, the fuel consumption was assumed to be 5% of the fuel consumption for the main engine.

For the results, the emissions per trailer are computed by dividing these total emissions per path by the number of trailers transported, given by the vessel's freight capacity Cap_{ij} multiplied by the utilization factor Ut_{ij}.

3.2 Method for Calculating External Costs

According to EU External Cost Handbook (CE Delft, 2019), the external costs are classified by Accidents, Congestion, Noise, Habitat, Air pollution, Climate Change and Well-To-Tank emissions costs. Each parcel is related to different negative externalities of the transportation sector and for each transport mode it assumes different impact magnitude and forms. Each external cost component had its negative impact on the environment and/or human health described in detail in Chapter 2, and the external cost values dependency to different parameters was presented in Table 2.1, such as the region where pollution is emitted or the polluter vehicle type.

In this thesis, external costs are presented as marginal costs, e.g., additional external costs as consequence of additional transport activity, linked to constant infrastructure capacity in the short run and extra infrastructure in the long run. External cost parcels described by the External Cost Handbook can be segregated in parcels induced by exhaust gas emissions, i.e., Air Pollution ad Climate Change costs, and parcels caused by the remaining externalities.

For emissions external costs, the methodology for computing the average Air Pollution cost $C_{AirPol,ij}$, in each path j part of the pair origin destination i, is obtained by equation below, multiplying the pollutant emissions $E_{ijk,SO_{2,}}$, E_{ijk,NO_X}, and $E_{ijk,PM_,}$ (in grams) by its respective costs c_{tonSO_2}, c_{tonNO_X} and c_{tonPM} (in EUR/ton of pollutant), respectively.

$$C_{AP,ijk} = \left(c_{tonSO_2} \cdot \ E_{ijk,SO_{2,}} \ + \ c_{tonNO_X} \cdot \ E_{ijk,NO_{X,}} + \ c_{tonPM} \cdot \ E_{ijk,PM_,}\right) \cdot \ 10^{-6} \qquad (29)$$

The air pollutant cost monetizes externalities caused by PM, NO_X, and SO_X emissions and this parcel is considered significant in every transport mode. The external cost per mass of pollutant emitted corresponds to marginal costs per EU member state, as extracted from the External Cost Handbook (CE Delft, 2019). The Handbook cost factors are based on the damage cost extracted from New Energy Externalities Development for Sustainability (NEEDS, 2008) method and latest studies (UBA, 2019) (Rabl, Spadaro, & Holland, 2014) and (OECD, 2014).

The marginal costs are considered independent on the density of the traffic flow, representing that emissions do not vary whether the vehicle is travelling in a thin or dense traffic flow area (kept the same location, speed, etc.). By the damage cost pricing approach, the factors correspond to costs paid by individuals to avoid – Willingness to Pay (WTP) – or to accept the damage caused by certain externality – Willingness to Accept (WTA). Several methods are used to estimate WTP, such as externalities valuation through transactions on other economic markets (revealed preference category) or through direct interviews/surveys of individuals (stated preference category).

For the last exhaust gas emission cost, the Climate Change cost $C_{CC,ij}$ is given by the multiplication of the equivalent $CO_{2\text{-eq}}$ emissions $E_{ijk,CO_{2-eq}}$ by the carbon price c_{tonCO_2}:

$$C_{CC,ijk} \ = \ c_{tonCO_2} \cdot \ E_{ijk,CO_{2-eq}} \cdot \ 10^{-6} \qquad (30)$$

Externalities caused by GHG emissions, the co-called Climate Change cost, make uses of the avoidance cost approach to determine its external cost valuation. By this method, current cost factors are defined to avoid having to incur costs in the future by preventing environmental deterioration defined by a certain policy target. An avoidance cost function is defined to estimate the supply of environmental quality, used to obtain the cost for increasing an extra degree of quality. Then, the lowest cost necessary to achieve the policy aim is estimated using this cost curve. This approach is especially suitable when externalities' damages are not clear, but some critics of this approach rely on the fact that policy targets do not consider individual country or region specifications.

In this thesis, the $CO_{2\text{-eq}}$ price adopted is exclusively based on the avoidance cost with regards to the limited temperature rises goals established in the Paris Agreement for a short and a long term. The avoidance cost was obtained by an extensive literature review made by the Handbook, grouping the cost in short and medium run (up to 2030) and long run (2040 to 2060). Table 3.12 presents the lowest, median, and highest carbon avoidance cost found. In this thesis, the reduction of one ton of CO_2 equivalent was adopted to be 100 EUR, representing an agreed value in the literature (CE Delft, 2019).

Table 3.12 – Climate avoidance costs in euros per ton of $CO_{2\text{-eq}}$ (CE Delft, 2019)

Term	Low	Central	High
Short and medium run	60	100	189
Long run	156	269	498

Another method for monetizing GHG emissions, as mentioned in the Literature Review, is the current EU regulations in the context of the Fit for 55 packages of actions, in which maritime transportation is introduced in the Emission Trading System (ETS). To have a comparative analysis of the EU carbon credit value traded in this system and the damage cost factor applied in this study, Figure 3.1 shows the evolution of carbon permits prices in EU ETS over 2022 (Trading Economics, 2022), highlighting that this price is volatile and subject to the influence of external events.

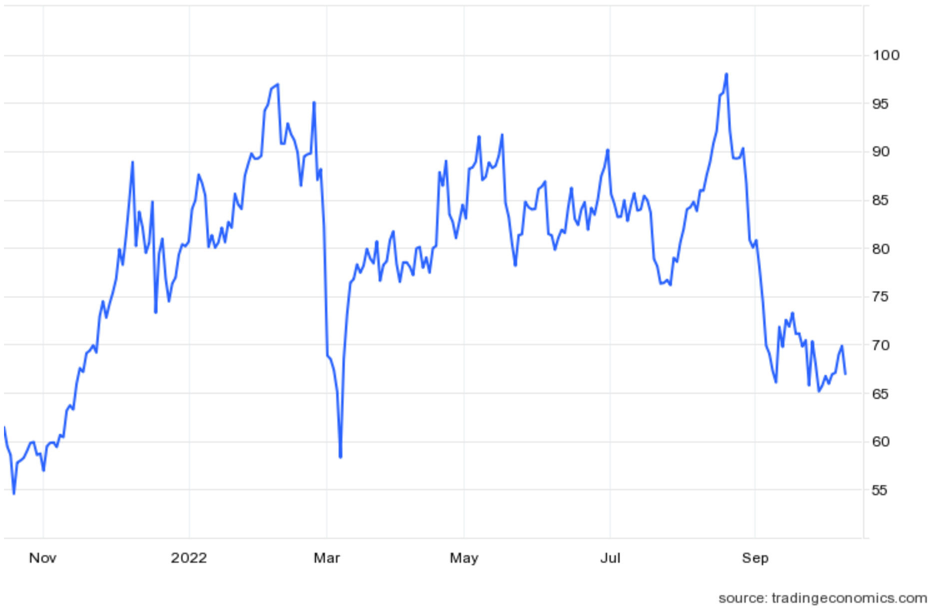


Figure 3.1 – Traded EU Carbon Permit prices in 2022

The remaining externalities – Accident, Noise, Congestion, Well-To-Tank (WTT) and Infrastructure costs – are simply computed by multiplying the distance travelled L_{ijk} in the link by its respective marginal cost, in cent-EUR/vehicle-km, and the region correction coefficient K_r:

$$C_{ext,ij} = K_r \cdot c_{ext} \cdot L_{ijk} \cdot 10^{-2} \quad (31)$$

The correction coefficient K_r corresponds to the value transfer applied to the input external costs factors extracted from the External Cost Handbook. The value transfer approach is a way to use input data, generated by the Willingness to Pay costs in a specific location and period, to other EU Member States realities. This approach is an attempt to estimate the valuation of externalities in countries where the primary data source is not available.

Even though Well-To-Tank (WTT) cost is associated with externalities caused by air pollutant emissions, WTT emissions are computed in this thesis and the simplified approach shown was adopted. The marginal WTT cost is virtually the same as the average cost, monetized in the same way air pollution was and, for the GHG emissions, it was adopted the shadow prices. However, energy related upstream emission factors were used for estimating emissions and then obtained the cost factors. For the road mode, marginal costs presented per vehicle-kilometer were computed using emission data from COPERT project.

Not only the air pollution cost was obtained from a damage cost approach, but also Accident and Noise cost factors, being a common method for the valuation of externalities (Botzen & Bergh, 2012). The marginal accident cost, only considered significant for road mode, is obtained from the accident risk (ratio between the number of casualties by the number of kilometers), cost per casualty (human, production, medical, administrative, material, and other costs) and risk elasticity. For road and rail modes, noise costs are determined by population density, existing noise levels and rime of the day, based on earlier calculations in (CE Delft; INFRAS; Fraunhofer ISI, 2011) and (INFRAS; IWW, 2004).

Like Accident and Noise costs, Congestion marginal costs are dependent on the traffic flow, and corresponds to high costs when a vehicle enters in a highly dense road. The social marginal congestion cost is computed by the approach presented in (Maibach, et al., 2000), considering different road types and levels of traffic intensity. The last external cost to be mentioned is the marginal infrastructure cost, associated with the renewal and maintenance of transport infrastructure. For road and rail modes, marginal costs were extracted from (INFRAS, CE Delft, 2019) and, for waterborne modes, this thesis does not cover infrastructure costs due to lake of information for all countries in analysis.

To properly compare different modes of transportation, the external cost is always divided by the cargo transported by vehicle. In the case of maritime transport, the cargo is function not only by the vehicle capacity Cap_{ij}, but also of its cargo utilization factor Ut_{ij}.

4. NUMERICAL TOOL AND VALIDATION

This chapter presents the numerical tool which has been developed based on the methodology previously described. In general, the transport network and emission database being defined, the output files are presented in a way to facilitate the understanding of the Sustainability Analyst (SA) functionalities and possibilities, and a validation of the outputs is presented.

4.1 Implementation in Numerical Tool

The software was developed and implemented in 2019 and some studies were published presenting the tool applied to a study case in Western Europe. The pollutant emission model was described in (Santos & Ramalho, Numerical Modeling of Air Pollutants and Greenhouse Gases, 2021a), including a study case with a limited geographic scope and route possibilities. Further extension of the previous study was carried out in (Santos & Ramalho, The Impact of the Internalization of External Costs in the Competitiveness of Short Sea Shipping, 2021b), including external cost internalization for the same geographical scope. Recently, the numerical tool was applied cruise ships emissions in the port of Lisbon (Abreu, Cardoso, & Santos, 2022). However, some changes were introduced in this software version:

- emission and external cost factors update based on current regulations,
- new methodologies for computing emissions,
- introduction of input parameters for vehicle definition,
- integration with IA software,
- new output files, including post-processing data.

Emission factors for rail transportation were modified to comply with new regulations applied by the European Commission. The energy-based emission factors for PM and NOx emissions were then described by Stage V of emission standards of engine for the propulsion of railway locomotives. Besides rail emission factors, external cost coefficients were revised according to original sources and updated truck parameters for emission computation were adopted.

The methodology for rail emission computations was previously restricted to locomotives with installed power of about 4,000 kW, without the dependence of some important train operational characteristics that impact on emission levels. The last software update makes use of energy factors derived from fleet-average data for rail transport of containers in 2018 that relates train speed to locomotive power demand (CE Delft, 2021). The power coefficients are given by Diesel and electric trains categories classified also by train length and cargo load, as presented in Chapter 3. This way the emission method can represent a broad range of rail networks, an important feature considering that shorter trains run on the Iberian Peninsula than in Western Europe.

Regarding maritime transportation, the first software version did not cover the fuel consumption originated from Power Take-Off systems, responsible for bow thruster and other auxiliary systems. Originally, power demand of the Ro-Ro ship in each operational profile was unknown and power loads from relevant literature were adopted. Even if usually the absence of information about shaft generators is balanced with a higher theoretical auxiliary engine load, SA is adapted to include this power source on the main engine fuel consumption in case the power balance is given by the shipowner.

An additional change introduced on the software was the differentiation of number of paths per pair O/D. Previously, the output was correctly given only if every pair O/D had the same number of possible paths, however, with the extension of geographical scope of the project, some transport chains were not reasonable to reach certain countries. For doing so, a new variable list was created for representing the number of paths in function of pair O/D and subsequent loops were adapted to a variable number of iterations.

Furthermore, new output files were introduced to reduce the time of post-processing in a second computational tool (usually Excel) and a better visualization of the results. The results of pollutant emissions and external costs per mode of transport were introduced in a new output file in which results are shown per pair O/D per country where the multiple paths cross. The output file containing major results from IA is now also read and the external cost internalization is done inside the numerical tool and the lowest total cost route is identified and plotted. With the matching between pair O/D and European region identification, maps containing the transport chain preferences are easily obtained, as will be shown in the following chapters.

The basic working principle of the Sustainable Analyst software is to identify which mode of transportation is used in a certain link, then a conditional statement drives to the appropriate numerical model to compute the link-specific emissions and external costs, storing these results in three kind of variables – total route results, results per transport mode, and results per country. The final route pollutant emissions and external costs are obtained by summing the specific results of each link, that composes a possible path connecting the origin to a certain destination. An outer loop runs for calculations to all remaining paths connecting the same O/D and the same procedure for the following pairs O/D.

Basically, the workflow structure consists of a log file, read by the program to internally identify input and output file names for further opening and reading of each data. The input data provides basic information about the transport network, vehicle's technical characteristics, external cost coefficients, transfer values, and emission factors. The transport network is defined by 3 different inputs:

- Network database: the file containing the relation between pair O/D, nodes sequence, vehicle technical properties identification, and path activity (active or inactive).
- Link sequence: file extracted from the Intermodal Analyst tool containing the set of links that composes a path.
- Link properties database: the file containing link-specific variables used on the numerical methods, such as link distance, link country, classification area (urban, suburban, or rural areas), speed, and link transport mode (road, rail, SSS, and IWT).

The vehicle's technical inputs are different for each mode of transportation, addressing the needs of each component of the numerical method for computing air emissions, while maintaining simplicity for changing vehicle characteristics in future studies. The transfer factors file presents the region coefficient per EU country to be applied to external costs. To conclude, the emission factors file gives information per mode and contains data about specific fuel consumptions and abatement technology emission effects.

After running the code, the output files present to each pair O/D, emissions, and external costs per transport mode and total per possible set of paths, per country, results in list format for better manipulation on Excel and, as already mentioned, the route with lowest internal, external, and total costs per destination. Figure 4.1 shows the basic workflow structure, presenting the input files, written in the log file, and, after running the SA program, the output files, as previously described.

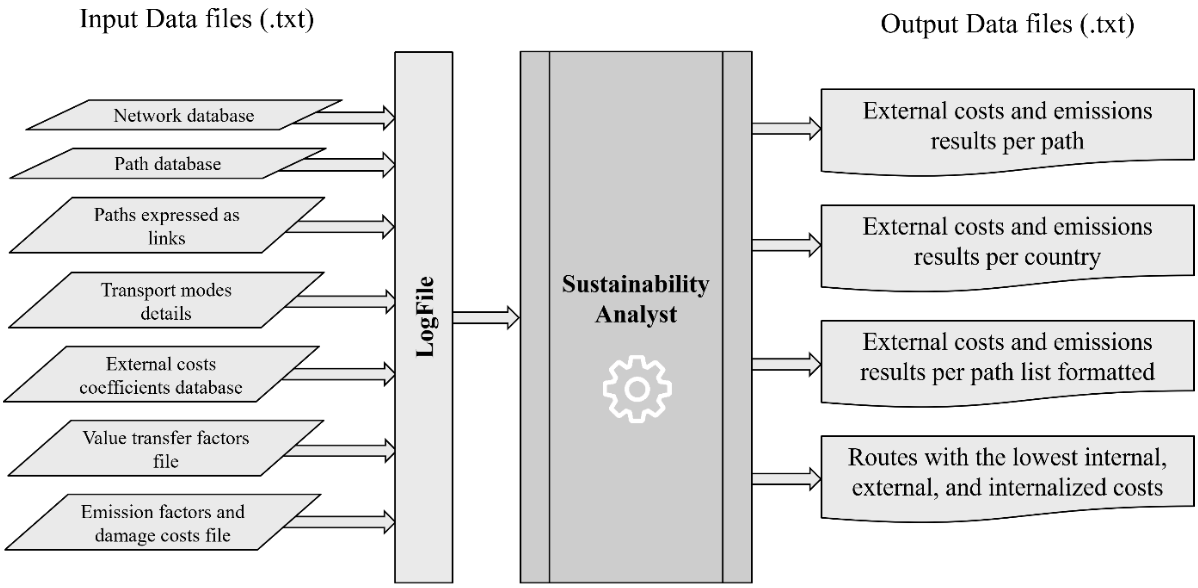


Figure 4.1 – Sustainability Analyst's new workflow

4.2 Validation of Numerical Tool

Outputs were first validated by implementing the numerical methodology previously described in Chapter 3 in a worksheet in MS Excel. Air pollutant emissions and appropriate external costs parcels per unit of cargo in every transport mode were analyzed in different paths for one pair O/D contained in the database, which complete definition is presented in the next chapter. Three paths connecting Porto, Portugal, to Stuttgart, Germany, were considered:

- Path 1: Road-only transport composed of 59 links.
- Path 2: Intermodal transport chain comprising road and rail mode and composed of 70 links.
- Path 3: Intermodal transport chain comprising road, inland waterway, and maritime modes and composed of 47 links.

Regarding maritime transportation, due to its complexity and diverse number of inputs, Path 3 was divided into two different scenarios regarding the vessel's technical characteristics. In Path 3A, the vessel was fueled with VLSFO and a combination of WS and EGR abatement technologies is adopted when navigating inside SECA. On the other hand, Path 3B considers a vessel propelled by a Tier 3 engine LNG-fueled. Table 4.1 presents the technical characteristics of each vehicle and other necessary inputs in each mode of transport.

Table 4.1 – Vehicle technical characteristics for validation

Truck	Train	Barge	RoRo vessel
- Travel time: DAY - Container weight: 30 ton - Truck type: Articulated - Truck class: 40 ton - Fuel type: DIE - Euro emission class: 5 - Specific fuel con.: 215 g/kWh - Engine power: 365 kW	- Emission Category: RLL - No abatement technology - Capacity: 40 FEU - Fuel type: Diesel - Train utilization: 100% - Length category: Long - Fuel consumption: 219 kg/h	- Directive stage: II - Fuel type: EN590 - Emission abatement technology: DPF+SCR - Rating speed: Medium - Cargo weight capacity: 1500 ton - Barge capacity: 50 FEU - Cargo utilization: 100% - Installed Power: 737 kW - Cruise Speed: 10 knots	- Length between Perpendiculars: 180 m - Breadth: 27 m - Draft: 7.5 m - Deadweight: 13,535 ton - Cargo capacity: 239 FEU - Vessel utilization factor: 100% - Engine Tier standard: 3 - Rating speed: Medium - Main engine power: 12,000 kW - Auxiliary engine power: 1,270 kW - Ship speed: 20 knots - Time at port: 6 h

Firstly, the database regarding link characteristics and the emissions factors was imported to Excel in the same way as it is read by the software. Then, the links identification number that composes a certain path is inserted and the sheet distributes the links IDs per transport mode worksheet, where the emission and external cost calculation methods are executed. In the end, the output is regrouped into one sheet in the same format as SA result files and the comparison can be done.

Regarding the road transport mode, Table 4.2 presents the difference between the software output and the Excel calculations per country. Both results were considerably similar with a maximum difference of 5 milligrams of SO_2 per FEU and 5 cents of euro per FEU for external costs.

Table 4.2 – Difference between Excel and SA outputs in Path 1

	Country	PT	ES	FR	DE	Total	Maximum
Emissions Trucks (/FEU)	NO_X (g)	5E-04	4E-03	3E-03	4E-03	3E-02	4E-03
	SO_X (g)	3E-03	3E-03	5E-03	1E-03	2E-02	5E-03
	$CO_{2\text{-eq}}$ (Kg)	4E-03	4E-03	2E-04	2E-03	3E-02	4E-03
	PM (g)	4E-03	3E-03	7E-04	4E-03	8E-03	4E-03
External Costs Trucks (€/FEU)	Congestion	3E-02	2E-02	4E-02	1E-02	2E-03	4E-02
	Accident	2E-02	2E-02	3E-02	4E-02	5E-03	4E-02
	Noise	3E-02	5E-02	1E-03	4E-02	2E-03	5E-02
	Air Pollution	2E-02	1E-02	2E-02	2E-02	1E-03	2E-02
	Climate Change	4E-02	3E-02	2E-02	3E-02	3E-03	4E-02
	Well-To-Tank	3E-02	3E-04	1E-02	2E-02	4E-03	3E-02
	Infrastructure	5E-02	2E-02	4E-02	2E-02	9E-04	5E-02
	Habitat	4E-02	5E-02	3E-02	5E-02	6E-04	5E-02
	Total	3E-02	3E-02	5E-02	2E-03	5E-03	5E-02

The software rail transport calculation performance could be noticed in Path 2 in which the absolute difference between both outputs is shown in Table 4.3 below. The order of magnitude for most of the results remains the same for road transport mode, with a slightly higher difference for the total Air Pollution cost. However, the relative difference in such a case is 0.2%, considered irrelevant for this study scope.

Table 4.3 – Difference between Excel and SA outputs in Path 2

	Country	PT	ES	FR	DE	Total	Maximum
Emissions Rail (/FEU)	NO_X (g)	4E-03	3E-04	4E-03	4E-03	6E-03	6E-03
	SO_2 (g)	2E-03	3E-03	5E-04	2E-04	3E-02	3E-02
	$CO_{2\text{-}eq}$ (Kg)	2E-03	1E-03	2E-03	5E-03	4E-02	4E-02
	PM (g)	1E-03	5E-03	2E-03	5E-03	4E-02	4E-02
External costs Rail (€/FEU)	Accident	3E-02	9E-03	3E-03	5E-02	4E-03	5E-02
	Noise	1E-02	4E-02	3E-02	2E-02	9E-04	4E-02
	Air Pollution	4E-02	2E-01	3E-01	3E-02	5E-01	5E-01
	Climate Change	1E-02	2E-02	3E-02	4E-02	3E-03	4E-02
	Well-To-Tank	4E-02	4E-02	4E-03	6E-03	6E-04	4E-02
	Infrastructure	5E-02	2E-03	2E-02	4E-02	2E-03	5E-02
	Habitat	5E-02	2E-02	4E-02	5E-02	1E-03	5E-02
	Total	6E-03	2E-01	3E-01	5E-02	5E-01	5E-01

To evaluate maritime modes inland waterways and maritime modes, Tables 4.4 and 4.5 present the absolute difference in IWT and SSS modes in Path 3A. Although results are a bit higher for emissions in IWT transport, the external cost difference is still in the order of cents of euros. In the case of maritime transportation, the outputs obtained in Netherlands and Portugal correspond to the emissions and external costs at the port.

Table 4.4 – Difference between Excel and SA outputs in Path 3A for IWT

	Country	DE	NL	Total	Maximum
Emissions IWT (/FEU)	NO_X (g)	3E-03	4E-03	6E-03	6E-03
	SO_2 (g)	2E-03	5E-04	3E-02	3E-02
	$CO_{2\text{-}eq}$ (Kg)	3E-03	5E-03	4E-02	4E-02
	PM (g)	5E-04	4E-03	4E-02	4E-02
External costs IWT (€/FEU)	Accident	3E-02	8E-03	2E-03	3E-02
	Air Pollution	2E-02	4E-02	2E-03	4E-02
	Climate Change	6E-03	2E-02	4E-03	2E-02
	Well-To-Tank	2E-02	2E-02	3E-03	2E-02
	Habitat	3E-02	4E-02	1E-03	4E-02
	Total	2E-02	3E-02	2E-03	3E-02

Table 4.5 – Difference between Excel and SA outputs in Path 3A for SSS

	Country	NL	PT	NA	Total	Maximum
Emissions SSS (/FEU)	NO_X (g)	4E-03	4E-03	4E-03	2E-02	2E-02
	SO_2 (g)	4E-03	4E-03	4E-03	2E-02	2E-02
	$CO_{2\text{-}eq}$ (kg)	4E-03	4E-03	1E-03	2E-02	2E-02
	PM (g)	2E-03	2E-03	2E-03	3E-02	3E-02
External costs SSS (€/FEU)	Air Pollution	4E-02	2E-02	5E-02	4E-03	5E-02
	Climate Change	3E-02	3E-02	3E-02	2E-03	3E-02
	Well-To-Tank	N/A	N/A	4E-02	3E-03	4E-02
	Total	3E-02	1E-02	4E-02	4E-03	4E-02

As mentioned before, an additional case was considered traveling the same path but with different vessel characteristics and the results for the maritime mode of transport can be seen in Table 4.6 below. Even changing some inputs, the maximum absolute difference has not changed for maritime transportation and the output per country has also slightly increased.

Table 4.6 – Difference between Excel and SA outputs in Path 3B for SSS

	Country	NL	PT	NA	Total	Maximum
Emissions SSS (/FEU)	NO_X (g)	4E-03	4E-03	4E-03	2E-03	4E-03
	SO_X (g)	4E-03	4E-03	2E-03	3E-02	3E-02
	CO_2 (Kg)	4E-03	4E-03	4E-03	5E-02	5E-02
	PM (g)	2E-03	2E-03	2E-03	5E-02	5E-02
External costs SSS (€/FEU)	Air Pollution	4E-02	2E-02	3E-02	5E-03	4E-02
	Climate Change	3E-02	3E-02	6E-03	5E-03	3E-02
	Well-To-Tank	N/A	N/A	4E-02	3E-03	4E-02
	Total	3E-02	1E-02	4E-02	6E-03	4E-02

A certain level of difference between both tools was accepted due to the software limitation regarding the number of digits printed on the output files and the considerable precision of Excel output. However, most of the results with high relative differences were the same considering the same number of algorithms truncated. Even so, some corrections were done on the software to match the Excel output and software output, for example, the fuel sulphur content on the road mode variation according to Euro standards and main engine fuel consumption considering PTO were corrected by simple adaptations on the code. In general, the differences obtained are minimal leading to the conclusion that the numerical tool Sustainability Analyst (SA) is satisfactorily validates and may be used on a systematic basis, something which would not be possible using a simple spreadsheet.

Online emission calculators were tested to validate the emission model. However, the websites present some assumptions that do not reflect reality in its complexity. For instance, in maritime transport, ports distances are uncertain, the ship type, cargo capacity and installed power are not inputs on the model. Regarding road mode, more accurate results were obtained with 10% variation on average compared to the software GHG emissions output for a specific route (Porto-Stuttgart).

5. CASE STUDY DEFINITION

This chapter details a case study designed to illustrate how external costs, and later internalization, affects route strategy, considering the major commercial partners of Portugal in the European Union. The geographic location of the set of pairs O/D is defined by establishing a single origin and multiple destinations, each one connected to the origin by a different set of possible paths. Each path is composed of a certain quantity of links that are related to a specific mode of transportation, in which vehicle characteristics are essential for determining external cost result behavior. Several routes combining different modes of transportation, intermodal terminals, and ship types are defined and characterized in this section. In addition, the vehicle's technical characteristics used as software input are defined for each mode of transportation.

5.1 Geographical Scope and Route Definition

In Chapter 4, exhaust gas emissions and external costs were computed for a specific route connecting a specific pair of O/D. These results depend directly on the geographical location of nodes contained on the transportation network because of the distance traveled, but also because unit external costs are a function of the country crossed by the route. In this case study many destinations will be considered, each one corresponding to the capital of a NUTS 2 (Nomenclature of Territorial Units for Statistics, level 2), considered representative of the entire region. The NUTS classification is a hierarchical system aiming to split up the EU and UK territories for socio-economic analysis and its second degree of specification represents basic regions of countries covered. Figure 5.1 presents the regions covered by the transportation network, including their NUTS 2 identification codes.

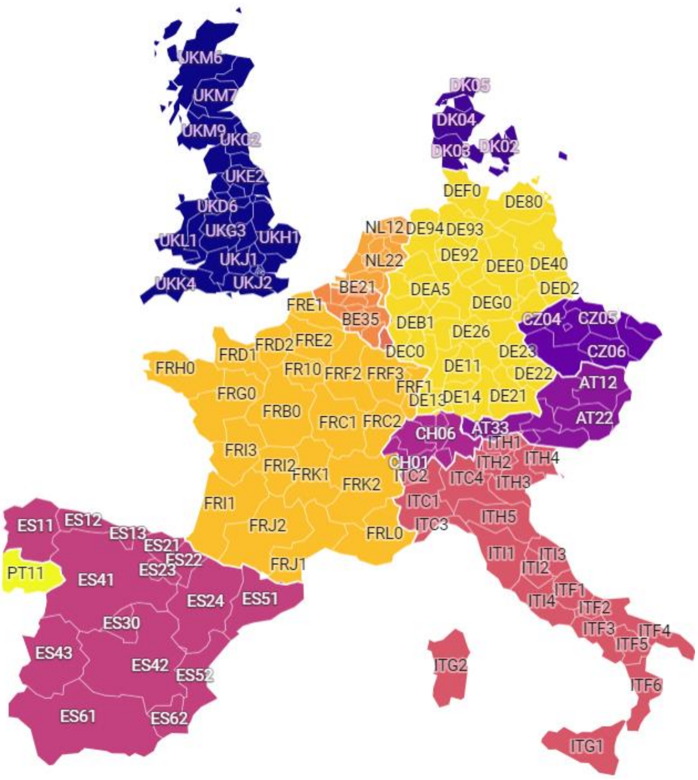


Figure 5.1 – NUTS 2 origin (PT11) and destination regions

The single origin Porto, capital of a highly intense industrial region of Portugal, is in the hinterland of port of Leixões, responsible for handling, on average, 20 million tons of goods per year, equivalent to 20% of the Portuguese export by sea (APP, 2022). Additionally, it is also a leader in the RoRo segment in Portugal, handling 1.3 million tons annually. On the other hand, destinations comprise the main commercial partners of Portugal in Europe. Altogether, the transportation network contains 188 destinations, covering 12 countries in Europe (Spain, France, Germany, Italy, Denmark, Switzerland, Czech Republic, Netherlands, Belgium, Luxemburg, Austria, and the United Kingdom). Only France (15%), Spain (14%), the United Kingdom (13.8%), Germany (10%), the Netherlands (5%), and Italy (2%) account for 60% of Portuguese exportation of goods in 2021 (BPstat, 2022) in a way that Portuguese international trade is properly represented by the geographical area covered in this case study.

Table 5.1 presents input paths, differing by mode of transportation combination, vehicle type, and/or intermodal terminal. The first path corresponds to the unimodal road and the other 25 routes are different combinations, always including road mode in door-to-door transportation. In some cases, just the intermodal terminal changes, as in paths 6 and 7, in which the road-rail transport chain passes through Entroncamento and Cacia, respectively. Different vessel types, i.e., container ship or RoRo, are applied on the same geographical route, defining different paths, such as paths 2 and 3; 11 and 13; 10 and 14.

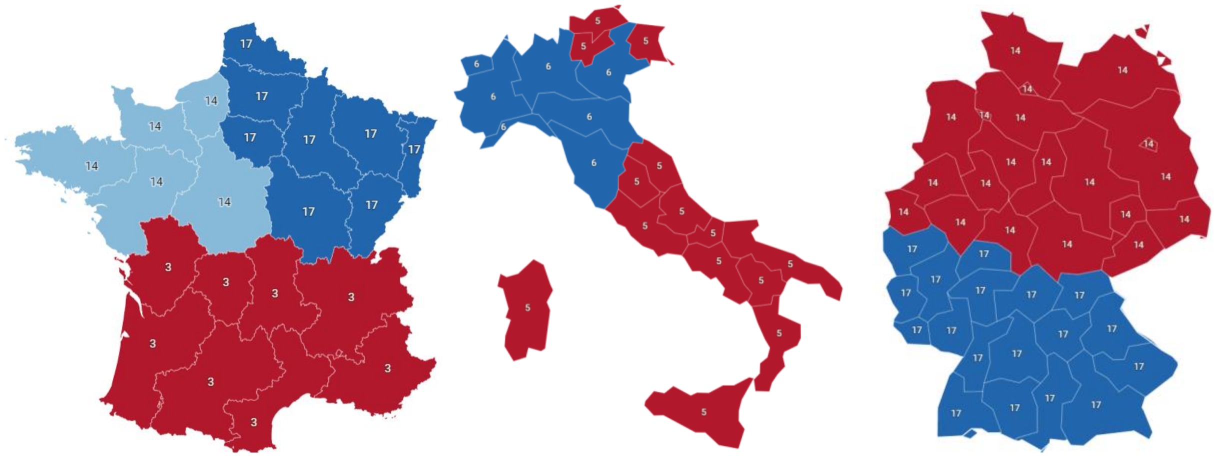
Table 5.1 – Set of paths description in modes of transportation, intermodal terminals, and vehicle types

Path	Modes	Terminals	Vehicles
1	Road	-	Truck
2	SSS Road	Rotterdam -	Container ship Truck
3	SSS Road	Rotterdam -	RoRo ship Truck
4	SSS Rail Road	Rotterdam Oberheim -	RoRo ship Train Truck
5	SSS IWT Road	Rotterdam Duisburg -	RoRo ship Barge Truck
6	Rail Road	Entroncamento -	Train Truck
7	Rail Road	Cacia -	Train Truck
8	SSS Rail Road	Rotterdam Mannheim -	RoRo ship Train Truck
9	SSS Rail Road	Le Havre Mannheim -	RoRo ship Train Truck
10	SSS Road	Le Havre -	RoRo ship Truck
11	SSS Road	Hamburg -	RoRo ship Truck
12	SSS Rail Road	Hamburg Wurzburg -	RoRo ship Train Truck
13	SSS Road	Hamburg -	Container ship Truck

Path	Modes	Terminals	Vehicles
14	SSS Road	Le Havre -	Container ship Truck
15	SSS Road	Marseille -	Container ship Truck
16	SSS Road	Valencia-Naples -	RoRo ship Truck
17	SSS Road	Setubal-Genoa -	Container ship Truck
18	SSS Road	Setubal-Genoa-Salerno -	Container ship Truck
19	SSS Road	Bilbao or Valencia -	Container ship Truck
20	SSS Road	Liverpool -	Container ship Truck
21	SSS Road	Tilbury -	Container ship Truck
22	SSS Road	Bristol -	RoRo ship Truck
23	SSS Road	Livorno -	RoRo ship Truck
24	SSS Rail Road	Hamburg Basel -	Container ship Train Truck
25	SSS Rail Road	Genoa Basel -	Container ship Train Truck
26	SSS IWT Road	Rotterdam Basel -	RoRo ship Barge Truck

Since 99.99% of all container transport performance on European inland waterways occurs in the six Rhine countries (Netherlands, Belgium, Germany, France, Switzerland, Luxembourg), and on the Danube, container transport by IWT is almost non-existent elsewhere (CCNR, 2021). For this reason, paths 5 and 26 comprise important segments in the Rhine River from Basel to Rotterdam, passing through Duisburg.

Each country comprises a different set of possible routes, and even in the same country, it is possible to have different route possibilities by macro-region. This is the case for regions in France, Germany, and Italy and the number of possible routes in each NUTS 2 in these countries can be seen in Figure 5.2. Northern Italy additionally considers path 15 to properly represent the port of Marseille activity area and Southern Germany includes paths 24 to 26, due to the proximity of the inland and rail terminal in Basel. These considerations allow a real representation of the realistically feasible routes for different geographical areas and not artificially limited by country borders. Additionally, not all paths presented in Table 5.1 are currently used (in fact, many do not currently correspond to technically possible routes) for the exportation of goods from Portugal and possible chain shifts are analyzed in different scenarios, as described in the following section.



(a) France (b) Italy (c) Germany

Figure 5.2 – Different number of possible routes for France, Italy, and Germany

5.2 Scenarios Definition

Different scenarios were simulated to evaluate the effect of the external cost of the transport chain preference on different operational conditions and routes. The first variable regards to how the route preference changes when new intermodal transport chains are considered. For doing so, the set of paths, so-called Scenario 1, represents existing routes in use nowadays, and after activation of new paths, the set of chains Scenario 2 is defined. Table 5.2 presents both sets of paths by country, in which routes with an asterisk represent the paths only considered in Scenario 1 and all the others were activated in Scenario 2, including the ones already marked with “X”.

Table 5.2 – Set of possible routes per country in route Scenarios 1 and 2

Path	Description	ES	FR	IT	LU	BE	NL	DE	CH	AT	CZ	DK	UK
1	Road	x*	x*	x*	x*	x*	x*	x*	x*	x*	x*	x*	x*
2	RoRo (Rotterdam) + Road		x		x	x	x	x			x		
3	Containership (Rotterdam) + Road		x*		x*	x*	x*	x*	x*	x*	x*	x*	
4	RoRo (Rotterdam) + Rail (Oberheim) + Road		x		x	x	x	x					
5	RoRo (Rotterdam) + IWT (Duisburg) + Road		x		x	x	x	x					
6	Rail (Entroncamento) + Road		x		x	x	x	x					
7	Rail (Cacia) + Road		x		x	x	x	x	x	x	x		
8	RoRo (Rotterdam) + Rail (Mannhein) + Road		x		x	x	x	x					
9	RoRo (LeHavre) + Rail (Mannhein) + Road		x		x	x	x	x					
10	RoRo (LeHavre) + Road		x		x	x	x	x					
11	RoRo (Hamburg) + Road		x		x	x	x	x				x	
12	RoRo (Hamburg) + Rail (Wurzburg) + Road		x		x	x	x	x					
13	Containership (Hamburg) + Road		x*		x*	x*	x*	x*		x*	x*	x*	
14	Containership (LeHavre) + Road		x		x	x	x	x	x				
15	Containership (Marseille) + Road		x	x					x				
16	RoRo (Valencia-Naples) + Road			x									
17	Containership (Setubal-Genova) + Road			x*					x*	x			
18	Containership (Setubal-Genova-Salerno) + Road			x									
19	Containership (Bilbao/Valencia) + Road	x*											
20	Containership (Liverpool) + Road												x*
21	Containership (Tilbury) + Road												x*
22	RoRo (Bristol) + Road												x
23	RoRo (Livorno) + Road			x					x				
24	Containership (Genova) + Rail (Basel1) + Road		x		x	x		x	x	x			
25	Containership (Genova) + Rail (Basel2) + Road		x		x	x		x	x	x			
26	RoRo (Rotterdam) + IWT (Basel) + Road		x		x	x		x	x	x			

* Transport chains considered in Scenario 1.

Scenario 1 routes were based on the mode of transportation most used in Portuguese international trade and the origin and destination of cargo handled in major Portuguese ports. Exportations of goods show that cargo mainly flows by road from Portugal and consequently, unimodal road (Path 1) were activated in all countries in this option. According to the Statistical Pocketbook 2021 about EU Transport (EC, 2021), the modal split of freight transport on land in 2019 is carried out mainly by road (85% of ton-km), followed by rail transport (12.7% of ton-km). Therefore, IWT and rail chains were not considered in Option 1 as these chains do not represent intense activity routes, and most certainly not for cargos originating in Portugal.

From port of Leixões' annual statistic reports, the port of Rotterdam is a leader in the number of containers handled, representing 27.7% of total cargo loaded and unloaded in 2019 and 27.1% in 2020 (APDL, 2020). Considering also that shippers do not usually use intermodal routes containing more than two modes of transportation, only the route containing a maritime path through Rotterdam and road transportation (Path 3) was activated to all countries on the set Scenario 1. Cargo flow from the United Kingdom is also carried out by routes through the port of Liverpool (Path 20) and Tilbury (Path 21), comprising around 5% and 2% of total cargo handled in Leixões in 2020. Regarding origin/destination port data does not include transshipment in different ports, and the last port in which cargo is handled before flowing to the end-door destination is unknown. Therefore, the port of Lisbon database was considered for determining that the port of Hamburg is the port representative of transportation of goods by sea between Portugal and Germany, covering destinations in most of the regions tested in Western Europe.

Moreover, the cargo capacity utilization in different vehicles is not readily available and differentiation regarding this parameter is done to properly compare rail, container ship, and RoRo transportation. Two conditions were assumed - 50% and 80% for all vessels and train lines - covering a sufficiently large range of values in which vehicles can operate. The lowest utilization factor is assumed by an estimation extracted from port data and the upper limit is a typical value in container ships. From the database provided on the port of Leixões website, it was possible to estimate the average utilization capacity of a typical RoRo vessel from the past 9 years by dividing the total cargo handled, in FEUs per year, by the number of RoRo calls per year and then, dividing it by a typical RoRo capacity in port of Leixões (434 TEUs). A similar approach was used for obtaining the port call size of container ships in port of Leixões, considering containers charged and discharged per year and the number of container ship calls per year. Using a linear regression for the ship capacity in function of the ship gross-tonnage, the average port call size is around 58%, based on the last 5 years' data.

The last variable considered is the adoption of trains propelled by electrical means, allowing an evaluation of the competitiveness of rail routes regarding Diesel and electric locomotives. In the European rail network, 60% of railway lines are electrified and 80% of traffic is running on these lines (EC, 2017). Although air-pollutant emissions are generated when traction current is generated, electric trains do not directly generate emissions locally, implying lower external costs on these routes and consequently their competitiveness regarding externalities. Table 5.3 summarizes the scenarios defined considering all previously mentioned variables and the results are presented considering such scenario definitions. Since the current scope of transport chains (Scenario 1) does not comprise chains with rail mode paths, the train type is not applicable for scenarios 1.1 and 1.2 in the table below.

Table 5.3 – Scenario description regarding route option, cargo utilization, and train type

Scenario	Cargo utilization	Train type
1.1	50%	N/A
1.2	80%	N/A
2.1	50%	Diesel
2.2	80%	Diesel
2.3	50%	Electrical
2.4	80%	Electrical

5.3 Vehicle Technical Characteristics

According to the software methodology presented in Chapter 3, general technical characteristics of the vehicle are required to compute air pollutant emissions and external costs in every mode of transportation considered. Aiming for a proper characterization of real-world conditions, vehicles choice was based on trucks, trains, and inland and ocean-going vessels currently applied on transport lines in Europe. After defining the most common vehicle type, required technical aspects are obtained from the database available online and, in case it is not available, approximations adopted according to the literature, always considering the selected transport mode characteristic in the line served.

For rail mode of transport definition, Rail Freight Corridors (RFCs) were established by Regulation 913/2010 for the selection, organization, and management of the European rail network to improve the competitiveness of international freight transport in Europe (IRG, 2022). Figure 5.3 presents the current rail network configuration, highlighting rail terminals connected by all nine rail corridors. In this study, rail axes connecting the port of Leixões to Entroncamento and Cacia rail terminals (RFC4) and the port of Le Havre to Mannheim terminal are included in Atlantic RFC, paths from the port of Rotterdam to Oberhausen and Mannheim rail terminals and from Genoa to Basel are included in Rhine-Alpine (RFC1) and from the port of Hamburg to Wurzburg intermodal terminal in Scandinavian-Mediterranean (RFC3).

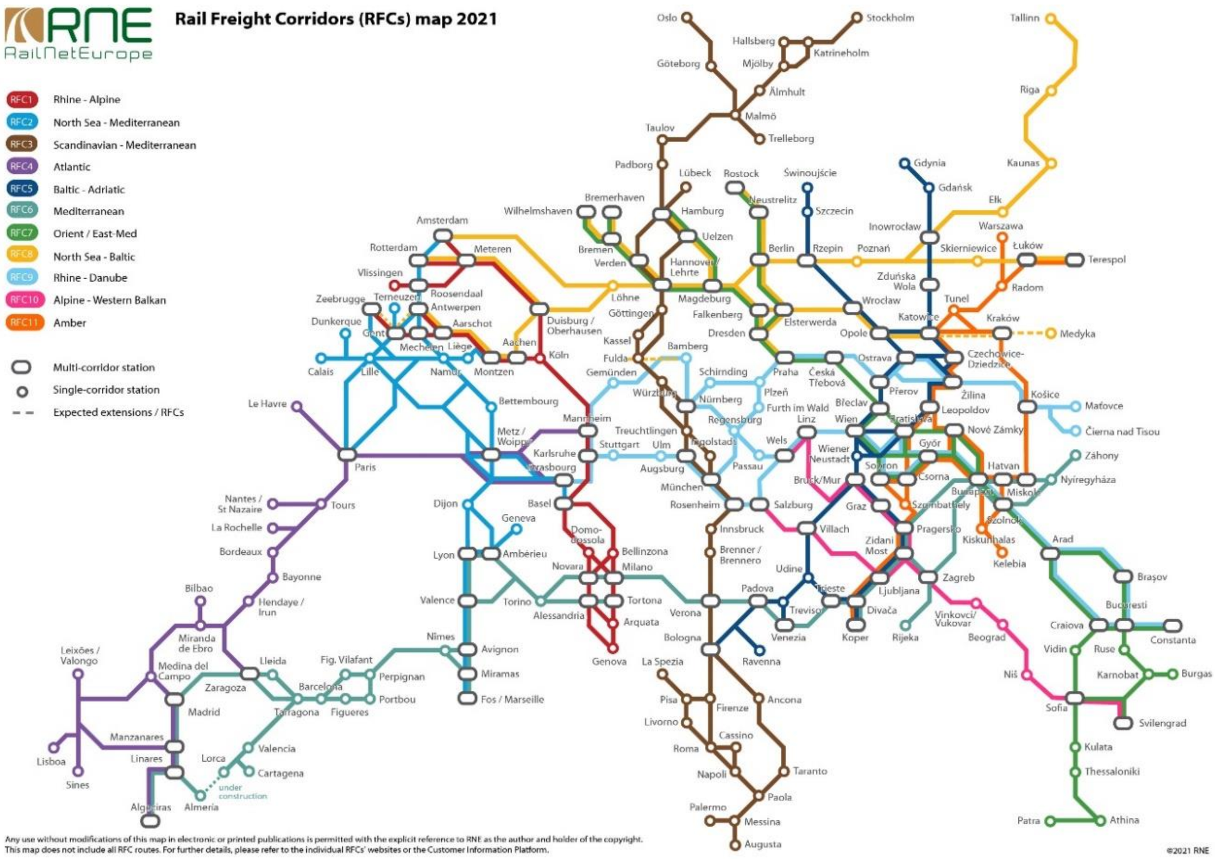


Figure 5.3 – Rail Freight Corridors in Europe

Information about trains' average speed and train length can be found in performance and annual statistic reports provided by each operator's websites (RFC Rhine-Alpine, 2021; Atlantic Corridor, 2020; TRT, 2019; FFE; RC, 2020; EC, 2020). Table 5.4 summarizes the relevant characteristics of railways used in each path of the transport network to compute emissions and external costs. From the observed data, it is possible to classify train about train's length and Gross Tonnage Weight, used to obtain the energy efficiency coefficient and compute demanded power. Notably, in the Iberian Peninsula container freight transport by railway presents shorter wagons and operate in lower speeds.

Table 5.4 – Train characteristics in different Rail-Freight Corridors

Path	From	To	Rail Freight Corridor	Average Speed [km/h]	Average Length [m]	Maximum Length [m]	Approx. capacity [FEU]
4	Rotterdam	Oberhausen	Rhine-Alpine	70.8	530	740	43
6	Leixões	Entroncamento	Atlantic	50	400	550	32
7	Leixões	Cacia	Atlantic	50	400	550	32
8	Rotterdam	Mannheim	Rhine-Alpine	70.8	530	740	43
9	Le Havre	Mannheim	Atlantic	63.3	700	740	57
12	Hamburg	Wurzburg	Scandinavian-Mediterranean	-	600	740	49

For road transport mode, a Class 8 long-haul truck was considered representative of trucks used in long distances road freight transport. This classification is based on the vehicle's gross vehicle weight rating (GVWR) used by manufacturers and applied to government guidelines and this class comprises trucks with a 40-ton gross weight truck. This category corresponds to the load limitation established by Directive 96/53EC on European roads (ACEA, 2015). Figure 5.4 presents the maximum permissible laden weight of a vehicle in EU road transport, in 2015, 2019, and 2020 (Eurostat, 2022)., indicating that most of the ton-km in road freight transportation after 2019 is carried out by trucks between 30 tons and 40 ton of gross laden weight.

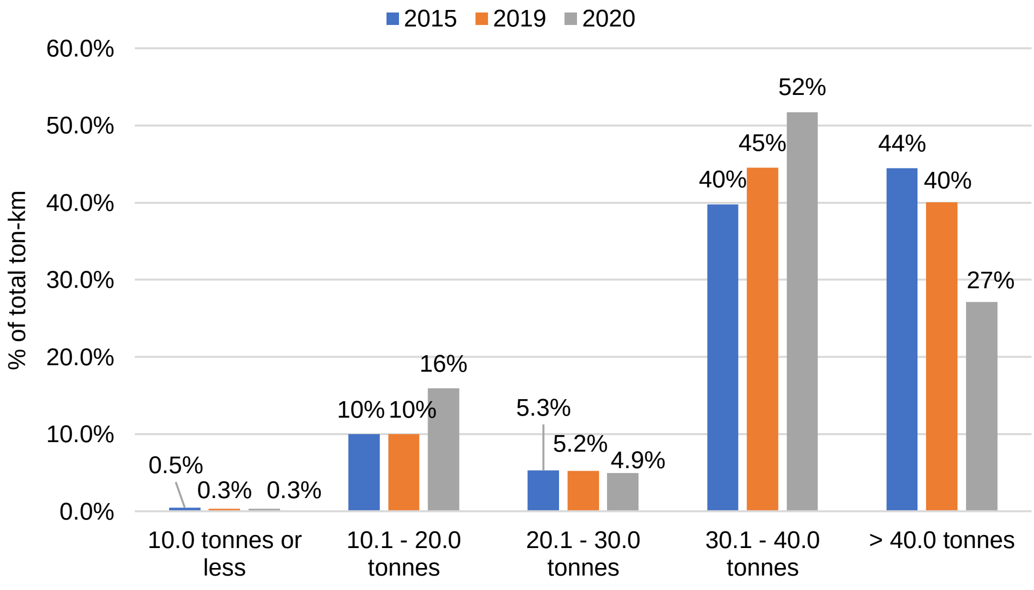


Figure 5.4 – Maximum permissible laden weight of vehicle, 2015, 2019, and 2020

Some of the paths included inland navigation, namely paths 5 and 26. The geographical area in which paths 5 and 26 take place is shown in Figure 5.5 (CCNR, 2021). According to the Central Commission for the Navigation of the Rhine (CCNR) in the most recent annual report of Inland Navigation in Europe, the average loading capacity or deadweight of a vessel in the Rhine fleet was around 1,500 tons in 2020, motivating the choice of a Large Rhine Vessel class.

Figure 5.5 – Inland Waterway Transportation in Rhine Basin from Basel to Rotterdam

The class of inland vessels is capable of transporting around 50 FEUs and the main technical characteristics can be found in (Interreg, 2018) and (Interreg, 2017), as presented in Table 5.5. Accordingly, this large multipurpose vessel mainly operates in the Rhine River stream and some examples can be found in free online AIS data providers, allowing efficient transportation of general cargo within containers along the basin. In this thesis, it is considered that the barge is equipped with a Diesel Particulate Filter (DPF) and scrubber to meet current environmental requirements.

Table 5.5 – Container inland vessel characteristics (Large Rhine Vessel)

Parameter	Value	Unit
Length	95	[m]
Breadth	11.4	[m]
Draught	2.7	[m]
Deadweight	1,500	[ton]
Cargo capacity	50	[FEUs]
Installed power	737	[kW]
Maximum speed	10	[kn]

The summary of truck and barge general technical characteristics used in the air pollutant emission calculation is shown in Table 5.6.

Table 5.6 – Truck and barge general characteristics for software input

Truck	Barge
- Travel time: Day	- Directive stage: II
- Container weight: 30 ton/FEU	- Fuel quality: EN590
- Truck type: Articulated	- Emission abatement technology: DPF+SCR
- Truck weight: 40 ton	- Rating speed: medium speed
- Fuel type: Diesel	- Cargo weight capacity: 1,500 ton
- Euro emission class: 5	- Barge capacity: 50 FEUs
- Specific fuel consumption: 215 g/kWh	- Cargo utilization: 100%
- Engine power: 365 kW	- Installed Power: 737 kW
	- Cruise Speed: 10 knots

Regarding maritime transportation, little information about RoRo lines is provided by ship operators and a typical vessel, operating in a line from port of Leixões to port of Rotterdam, was used for characterizing every other path travelled by the same ship type. Regarding container ships, a more accurate approach was adopted by searching vessels in actual container lines connecting Portugal to major European ports. Among 12 regular container lines, operated by 7 different shipping companies, vessel names and IMO number of container ships in operation were found on the operator's websites. Some vessels or twin vessels are applied in more than one container line, or in the same line, the vessel calls different ports. Table 5.7 shows the vessel type and identification used in the mentioned port of calls. The vessel identification is used on the next table for presenting the ship's technical aspects.

Table 5.7 – Vessels adopted to each port of calls

Vessel	Vessel Type	Port of Calls
Vessel 1	RoRo	Rotterdam, Le Havre, Hamburg, Valencia, Bristol, Livorno
Vessel 2	Containership	Rotterdam
Vessel 3	Containership	Le Havre, Hamburg
Vessel 4	Containership	Setubal, Marseille, Genoa, Salerno
Vessel 5	Containership	Bilbao, Valencia
Vessel 6	Containership	Liverpool
Vessel 7	Containership	Tilbury

Afterward, the technical information of a representative ship of each line was obtained from the *Scheepvaartwest* website. The ship information about main dimensions (draught, length between perpendiculars, mounded breadth) and operational aspects (cruise speed, capacity, and engine) are required parameters for running the emission method and are presented in Table 5.8.

Important features shown in the table above partially explain results behavior, such as ship capacity and installed power for the ensemble of paths through the ports indicated. Firstly, the RoRo ship has notably a lower cargo capacity than container ships applied in every other route. Regular lines connecting short distances in Portuguese, Spanish, and North African ports also apply to vessels with limited capacity compared to those operating in North Sea ports but sails in short sea distance. On the other hand, large container ships carry out transportation through Rotterdam and Mediterranean ports in France and Italy.

Table 5.8 – Ship's particulars used in different port calls

Particulars	Vessel 1	Vessel 2	Vessel 3	Vessel 4	Vessel 5	Vessel 6	Vessel 7
Length bet. Perpendicular [m]	195.4	158	131	166	127	125	142
Breadth [m]	26.2	27.2	22.8	27.4	19.4	22.5	23.4
Summer Draft [m]	7.4	13.6	8.7	10.9	7.36	8.71	8
Deadweight [t]	13,625	15,952	12,558	23,286	8,496	11,252	13,172
Capacity [TEU]	434	1,600	924	1,696	706	804	1,036
Engine tier	2	2	2	2	2	2	2
Speed rating	MS	SS	MS	SS	MS	MS	MS
Main engine power [kW]	5,905	12,640	9,600	18,820	7,195	8,400	9,000
Auxiliary engine power [kW]	2,540	2,400	1,500	3,540	860	2,036	1,650
Power Take-Off [kW]	3,750	3,400	1,700	900	1,315	2,238	2,500
Cruise speed [kt]	15	20	18.3	20.5	17.9	18.5	18.5

The loads of the main engines, expressed as percentages of MCR, auxiliary machinery, and Power Take-Off system in each operational profile are also a piece of important information for computing fuel consumption. Since it was obtained from the RoRo operator the power balance of the ship, real utilization percentages are used in Vessel 1, also considering the information of shaft generator load conditions. For the container ship, typical values found in the literature were applied. As mentioned in the methodology section, usually basic information about ship energy balance disregard shaft generator usages, considered not significant compared to main engine power. A summary of load factors is found in Tables 5.9 and 5.10 below.

Table 5.9 – Power load for container ships per operational profile

Machinery	Sea	Port	Maneuver
Main engine	100%	0%	0%
Auxiliary engine	30%	50%	40%
Power Take-Off	0%	0%	0%

Table 5.10 – Power load balance for RoRo per operational profile

Machinery	Sea	Port	Maneuver
Main engine	100%	0%	0%
Auxiliary engine	0%	7%	84%
Power Take-Off	60%	0%	100%

6. NUMERICAL RESULTS

The theoretical background of the numerical model for exhaust gas emissions and external cost calculations in the transportation chain was detailed described in Chapter 3 and technical aspects of the implementation were covered in Chapter 4. Chapter 5 presented the particularities and scenarios of the case study and in this chapter the software's results are presented.

Considering the complexity and size of results obtained for each air pollutant and external cost parcel, in each mode of transportation, a summary of the main results is presented in the form of maps, allowing to take important conclusions along the objectives of this thesis. Mainly, results are based on maps and graphs and data are used in some cases to explain their behavior in specific regions.

6.1 Externalities Assessment

The first set of maps in this section is based on the preferable route, considering only the external cost related to the complete transportation of goods from Porto to different regions in Europe. For a certain pair O/D, the total external cost comprises every externality parcel generated by all modes of transportation applied on the transport chain. Then, the total external cost is computed for every transport chain option available on the transportation network to a certain destination and the conclusion of which chain has the lowest negative impact on the environment and human health can be drawn for each specific region. Among many other factors here presented, chain preference is primarily influenced by the set of possible transport chains defined by each country, travelled, distances and vehicles' technical characteristics, as defined and justified in the previous chapter.

Firstly, the chain preference map, regarding total external costs, is presented for Scenario 1.1, in which the set of available routes comprises just existing possibilities to transport cargo from Portugal, cargo capacity utilization of vessels and trains was set at 50% and only Diesel propelled locomotives are used in railways. In Figure 6.1, the preferable transport chain can be identified by its numbering presented in Table 5.2 and the color can indicate the region where a certain chain is predominant, i.e., chain competitiveness scope area. Table 6.1 summarizes the results shown in the preference map of Scenario 1.1, presenting the number of regions and land area corresponding to the preferable path chosen. The areas shown were computed from the database of land cover per NUTS 2 region in Europe in 2018, extracted from Eurostat (Eurostat, 2021).

Under these restrictions, the only-road chain preference area (Path 1, in yellow) extends through Spain, a large part of France, and Switzerland. The lack of competitiveness of well-known sustainable modes of transportation in the chain (rail and maritime transportation) can be explained by the geographic proximity of the North of Portugal to these countries, in which no port or rail terminal is sufficiently close to the destination to overcome the advantage of a short road distance. Indeed, in Spain, besides the NUTS region where the port of Bilbao is located (ES21), Path 1 was preferred in all other regions instead of Path 19, which included the use of container ship. Furthermore, the second Spanish port considered, the port of Valencia (also path 19), is not used due to the environmental impact related to a long distance on the maritime path for contouring the Iberian Peninsula.

The only-road transportation can be also evaluated by the largest preference area, around 40% of the geographic scope on the map, and the largest influence of a maritime chain from port of Rotterdam (path 3) corresponds to 18% of the total area.

Table 6.1 – NUTS and areas in Scenario 1.1: current routes (50% cargo capacity utilization)

Path ID	Description	#NUTS	%NUTS	#Area [1000 km^2]	%Area
1	Road	33	18%	898	40%
3	Containership (Rotterdam) + Road	53	28%	390	17%
13	Containership (Hamburg) + Road	39	21%	412	18%
17	Containership (Setubal-Genoa) + Road	22	12%	305	14%
19	Containership (Bilbao) + Road	1	1%	7	0.3%
20	Containership (Liverpool) + Road	18	10%	128	6%
21	Containership (Tilbury) + Road	22	12%	102	5%
	Total	188	100%	2,242	100%

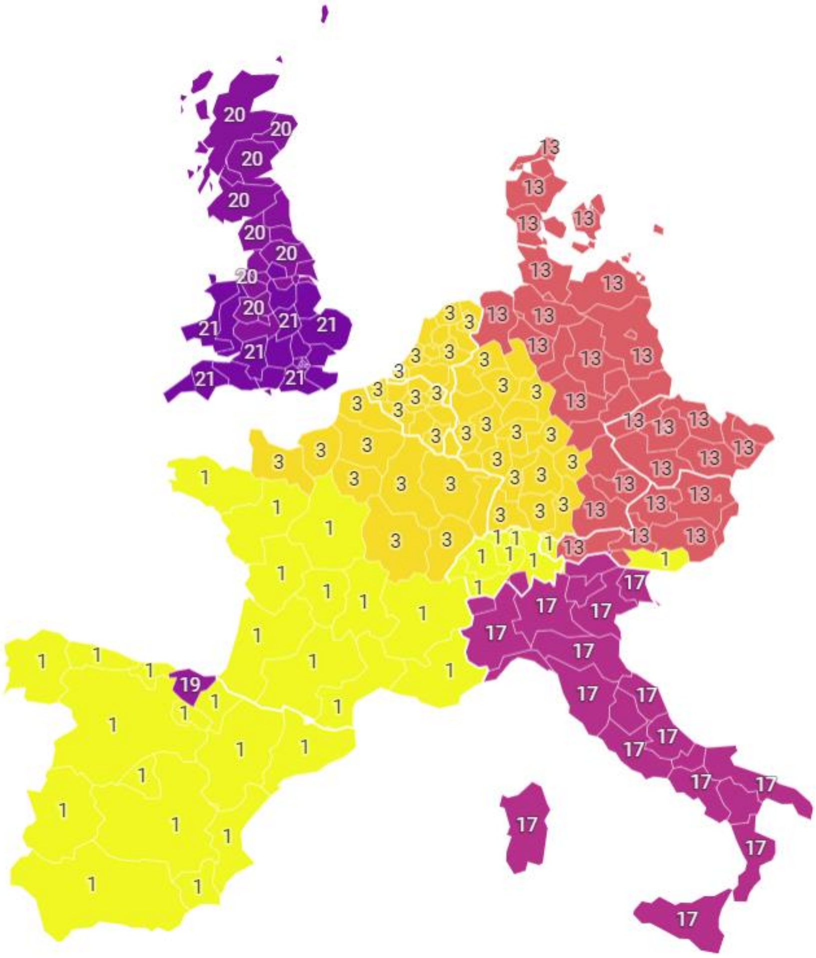


Figure 6.1 – Preferred transport chain in scenario 1.1: current routes (50% cargo capacity utilization)

An unusual road route preference is noticed in the Klagenfurt region (AT21), in which road is chosen rather than maritime transport from the port of Hamburg (Path 13). Even though the maritime path presents many advantages in the Congestion and Infrastructure costs, Well-to-Tank external cost in Path 13 is 8 times more expensive than the WTT cost in the most competitive only-road path (path 1) and consequently, the total external cost is slightly higher (0.3% higher).

The port of Genoa is the first Mediterranean port that can be noticed on the map due to the increasing competitiveness of SSS. The preferable path consists of a route departing from the port of Leixões, with a call to port of Setubal before following the way to the Italian port. In Northern Italy, even considering that NUTS in this region present shorter road distances than the navigation leg to port of Genoa, the maritime transport has presented a more competitive external cost.

Intermodal transport chains presented a considerable reduction in externalities related to destinations in Western and Central Europe, represented by areas where paths 3 and 13 are preferable, i.e., the total external cost is lower than only-road mode. The port of Rotterdam has consistent participation in the chain preference in Western Europe, covering Belgium, the Netherlands, Luxembourg, Northeast France, and Western Germany. On the other hand, the port of Hamburg covers important areas in East Germany, Denmark, Czech Republic, and Austria. The percentage reduction by using the port of Rotterdam and port of Hamburg, compared to Path 1, is presented in the map in Figure 6.2. On average, the total external cost has been decreased by -44% and -40% by adopting maritime Paths 3 and 13, respectively, and higher reduction percentages can be noticed close to NUTS regions located close to ports, in the Netherlands and in Northern Germany, getting up to -68% lower costs. For countries where path 3 has better performance than path 13, routes presented a slightly higher cost than chains through Rotterdam, comprising, on average, approximately 10% higher values. This fact indicates that the environmental impact of adopting either Rotterdam or Hamburg is relatively similar, mainly because these ports are geographically located in proximity. The general conclusion is that even in the current situation, with existing containership routes, intermodal solutions based on SSS may achieve very large reductions in external costs.

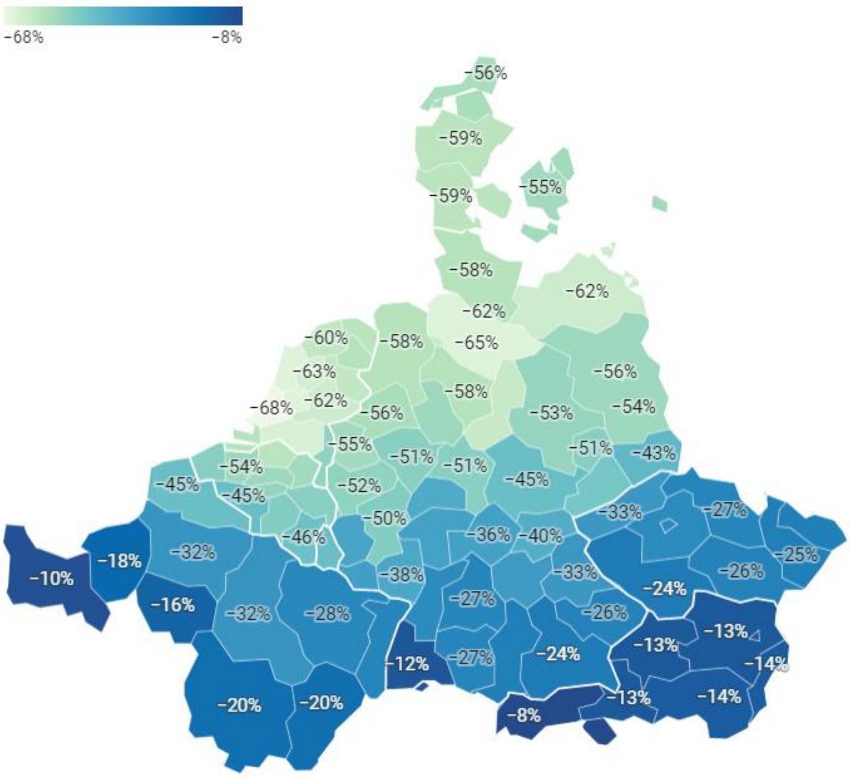


Figure 6.2 – Reduction percentage in external costs between only-road mode and preferable chain through port of Rotterdam or Hamburg

Figure 6.3 presents the transport chain preference in Scenario 2.1 following the criteria of lowest total external cost. In this scenario, the full scope of intermodal routes is adopted, comprising additional chains that make use of rail terminals and ports not commonly used nowadays. Trains and ships are set to 50% of total cargo capacity and train locomotives are Diesel propelled. Major differences are noticed in the region previously designated by paths 3 and 13, with the presence of new ports. Table 6.2 summarizes the number of NUTS and cover area for Scenario 2.1, presenting a reduction in the area percentage of road only modal compared to the scenario with current transport chain scope of routes.

Table 6.2 – NUTS and areas in Scenario 2.1: full scope of intermodal routes (50% cargo capacity utilization)

Path ID	Description	#NUTS	%NUTS	#Area [1000 km^2]	%Area
1	Road	20	11%	639	28%
3	Containership (Rotterdam) + Road	27	14%	109	5%
13	Containership (Hamburg) + Road	34	18%	345	15%
14	Containership (Le Havre) + Road	41	22%	539	24%
15	Containership (Marseille) + Road	2	1%	57	3%
17	Containership (Setubal-Genova) + Road	16	9%	202	9%
18	Containership (Setubal-Genova-Salerno) + Road	7	4%	113	5%
19	Containership (Bilbao) + Road	1	1%	7	0.3%
20	Containership (Liverpool) + Road	18	10%	128	6%
21	Containership (Tilbury) + Road	22	12%	102	5%
	Total	188	100%	2,242	100%

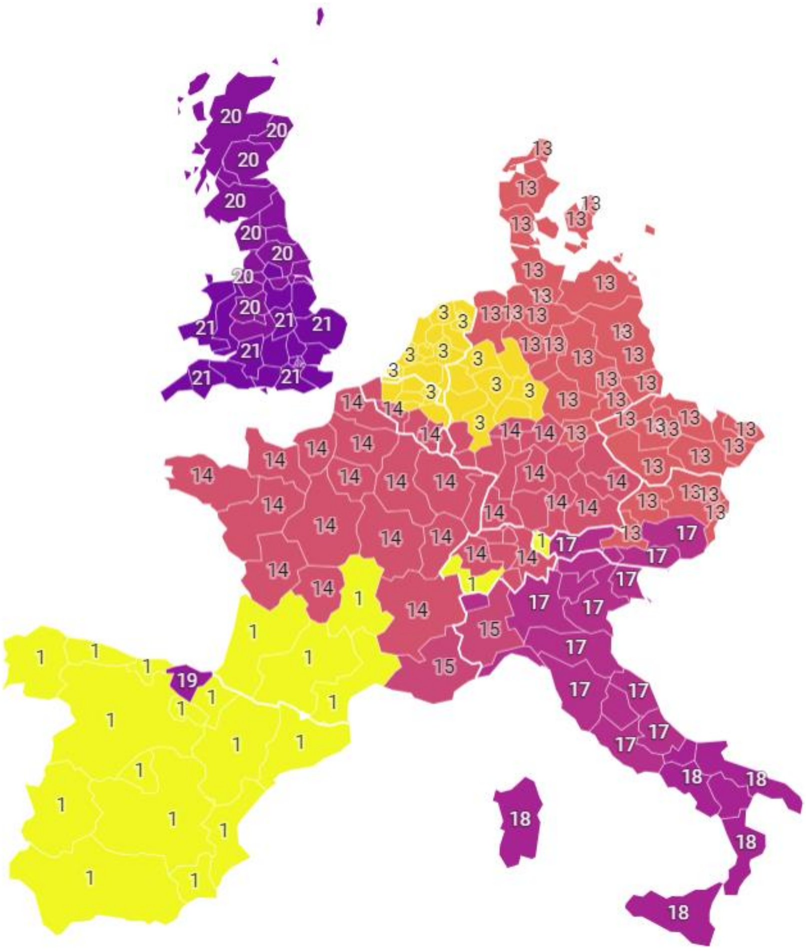


Figure 6.3 – Preferred transport chain in scenario 2.1: full scope of intermodal routes (50% cargo capacity utilization)

The Spanish set of transport chains in Scenario 2.1 was not modified from Scenario 1.1, implying the same map configuration as the previous map. The same configuration is also noticed in the United Kingdom, representing that an additional route to the port of Bristol is not competitive in terms of externalities. However, an important change in the configuration is noticed in France, in which the only-road preference area is reduced, giving place to new intermodal routes through important French ports. The unimodal route (Path 1) was replaced in central France by the port of Le Havre (Path 14), which also extended its influence over the Northeast region, previously occupied by the port of Rotterdam (Path 3), and the port of Marseille (Path 15) is present on the Southern region.

The port of Le Havre extends itself beyond France - in Belgium before identified by routes through the port of Rotterdam; in Southern Austria and Southwestern Germany, previously identified as port of Hamburg; and regions in Switzerland, previously only-road route. The predominance of Le Havre can be partially explained by the vessel used in this route, comprising a container ship with higher cargo capacity. Even though a greater installed power is necessary to maintain the cruise speed, the cargo capacity can provide an economy of scale in terms of fixed externalities per unit of cargo.

In Italy, the hegemony of routes from the port of Genoa in Figure 6.1 was ended by routes to the port of Salerno (Path 18) in Figure 6.3, reinforcing the importance of maritime transport as a sustainable mode. Regions in Southern Italy were reached by a road path from the port of Genoa in Scenario 1.1, however, considering an additional route, cargo is taken directly to the port of Salerno in Scenario 2.1. Therefore, this results in a shorter road distance by using a port geographically closer to the destination. The smallest environmental and human health impacts for routes from the North of Portugal to Piemonte occur for the route from port of Leixões to port of Marseille, showing that the preferences for specific paths are not limited to country borders.

In Scenario 2.1, Geneva (CH01) and Vorarlberg (AT34) regions have adopted Path 1, even being within an intermodal preference area. Figure 6.4 presents the difference in all external cost parcels from intermodal transport (Path 14) to road-only route (Path 1), in which negative columns represent savings when adopting a intermodal route and positive columns indicate additional costs Notably, the intermodal path presents advantages in most of the externalities, which summed usually compensate for the high Well-To-Tank cost associated with the maritime route. However, the equilibrium is broken whether the Congestion cost is not favorable to the intermodal route, and its variation is related to the traveled distance and road classification. For instance, the adoption of the intermodal route has resulted in -69 EUR/FEU of savings, compared to only-road mode, to transport to Bern, and to reach the previous region, Geneve, intermodality is 17 EUR/FEU more expensive than only-road, due to the fact that only-road is favored by shorter road distances to Geneve. Table 6.3 summarize the absolute congestion costs in each region.

Table 6.3 – Congestion cost in intermodal and only-road routes (in EUR/FEU)

Route	Geneva	Bern	Difference
1	160	214	54
14	177	145	-32
Difference	-17	69	

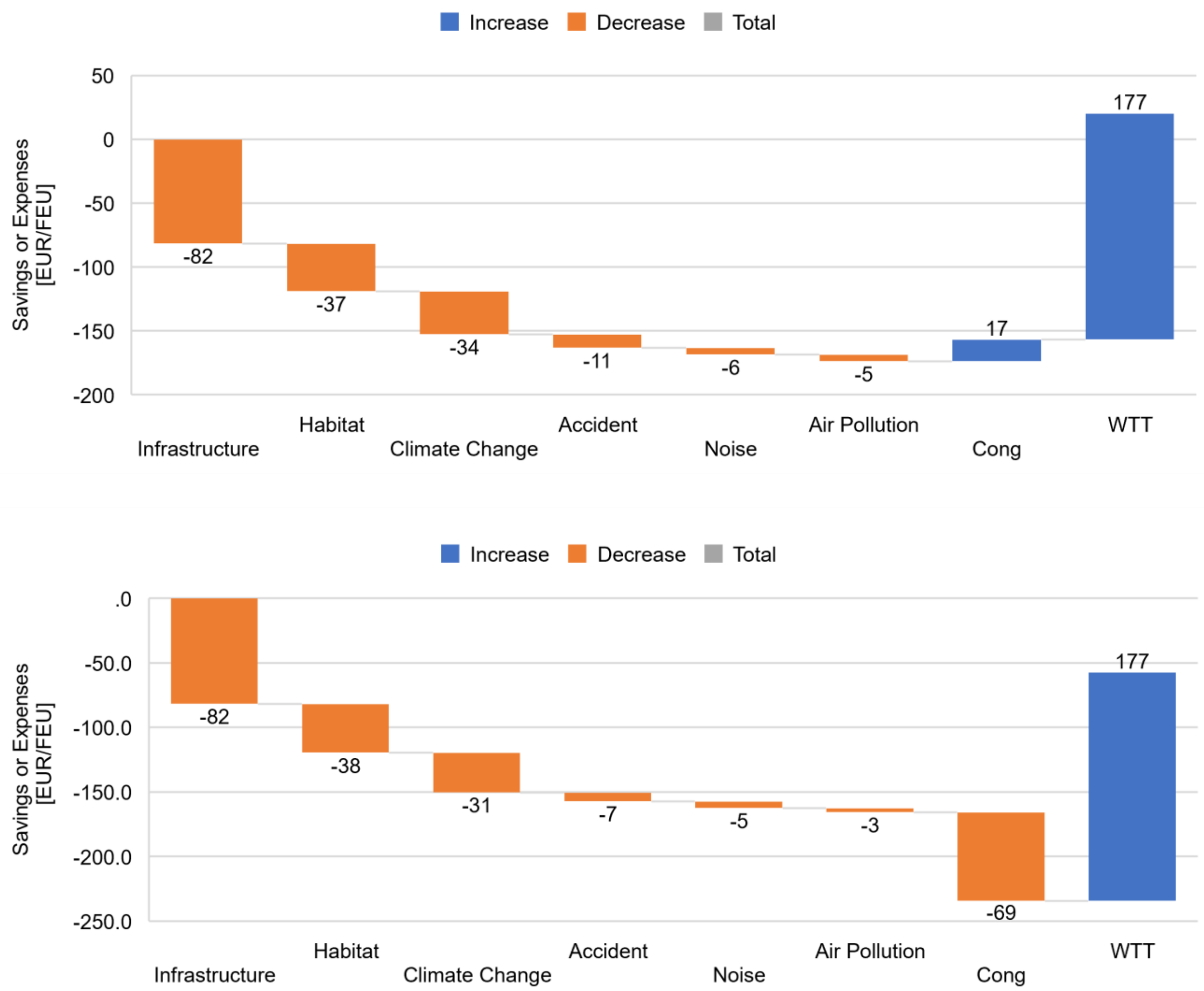


Figure 6.4 – External cost differences between Path 1 and 14 in Geneva (above) and Bern (below)

Figure 6.5 presents the impact on the chain preference map by an increased cargo capacity utilization in vessels and trains, set to 80%, considering the existing transport network in Scenario 1.1, defining the second variation of current chain scope Scenario 1.2. The new operational configuration below originated a more continuous map, compared to Scenario 1.1, in which previously adopted intermodal chains have expanded their influence and new chains are more competitive over only-road mode.

Table 6.4 presents the number of NUTS regions and respective area in each preferable path noticed in Scenario 1.2. As can be seen in the table, the area of influence of road-only transportation has increased to 31% compared to 28% in the previous situation (Scenario 2.1). However, the situation has improved when compared to situation using the same transport chain scope and a lower cargo utilization factor (Scenario 1.1) when road participation was 40% of total area. This represents that the current intermodal transport network can present a better performance depending on the increasing cargo capacity.

Table 6.4 – NUTS and areas in Scenario 1.2: Current routes (80% cargo capacity utilization)

Path ID	Description	#NUTS	%NUTS	#Area [1000 km^2]	%Area
1	Road	19	10%	706	31%
3	Containership (Rotterdam) + Road	51	27%	450	20%
13	Containership (Hamburg) + Road	45	24%	461	21%
17	Containership (Setubal-Genova) + Road	28	15%	344	15%
19	Containership (Bilbao/Valencia) + Road	5	3%	51	2%
20	Containership (Liverpool) + Road	18	10%	128	6%
21	Containership (Tilbury) + Road	22	12%	102	5%
	Total	188	100%	2.242	100%

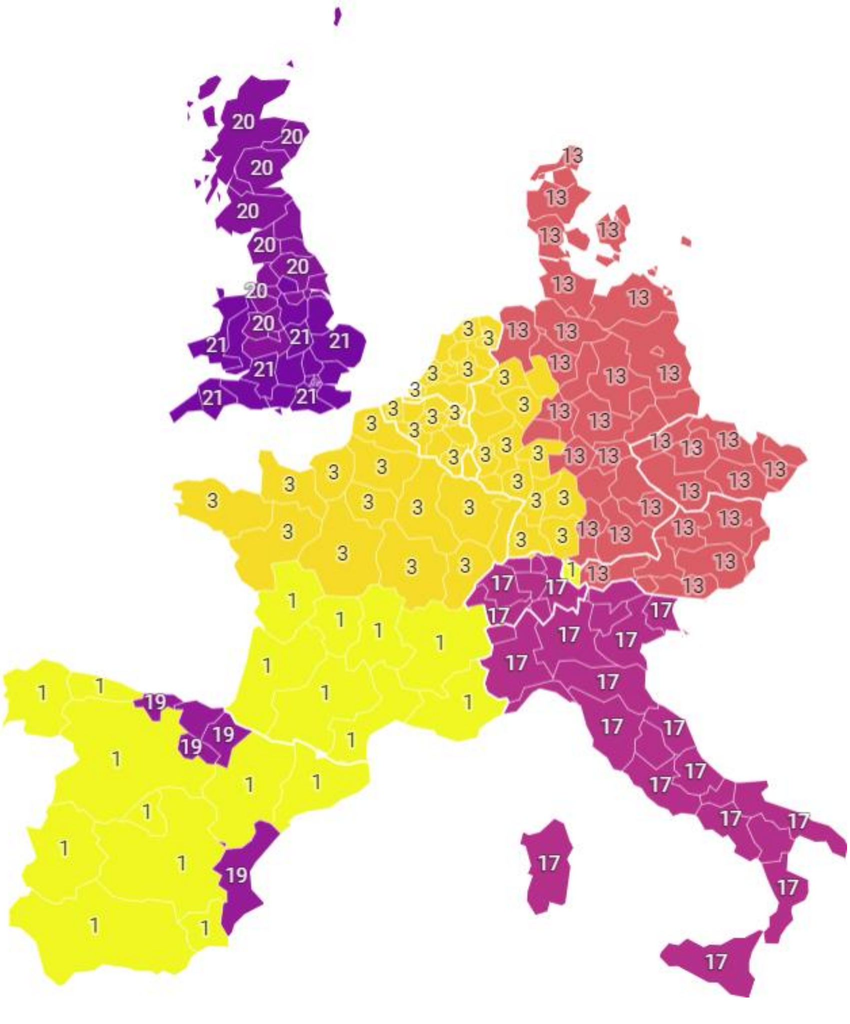


Figure 6.5 – Preferred transport chain in scenario 1.2: Current routes (80% cargo capacity utilization)

On Spain's southeastern coast, the total external cost of the route through the port of Valencia (Path 19) is 281 EUR/FEU by using 80% of containership cargo capacity, which represents -32% lower value than the case with 50% cargo utilization factor (415 EUR/FEU). Even though all other externalities related to maritime transport (Air Pollution and Climate Change costs) have decreased, Well-to-Tank cost was the major contributor to the worse performance, but it was diminished from 292 to 182 EUR/FEU in the new condition. Therefore, the external cost of only-road mode (294 EUR/FEU) became larger than Path 19 externalities, and this intermodal chain became more competitive.

The situation presented in Spain exemplifies the cargo capacity utilization effect over externalities, and it can be extended to all other regions. Considering that the route is kept the same and externalities dependence is restricted to distance traveled and unit external costs (countries crossed), these external cost components are directly reduced by the inverse of the increment rate of cargo utilization factor. The total external costs are compared by dividing them by the number of units transported, and whether the externality does not vary with other variables, a positive effect is direct. Externalities related to exhaust gases are not decreased by the same percentage of cargo occupation increment due to the increasing fuel consumption under a higher effective power demand, even though the economy of scale is still favorable. The major responsible for maritime environmental performance degradation is significantly affected by the increasing number of cargo units onboard. Savings in Well-to-Tank cost have a strong influence on the transport chain preference.

In Scenario 1.2, existing intermodal transport chains through the port of Rotterdam (Path 3), Hamburg (Path 13), and Genoa (Path 17) have the least environmental impact on a larger geographical area due to the improved maritime performance previously mentioned. Compared to Scenario 1.1 (Figure 6.1), the port of Rotterdam has extended to more regions in Northern France (Orleans, Nates, and Rennes regions) and the port of Hamburg has offered a more suitable transport solution in terms of externalities in a greater extension of Germany (Nuremberg, Wurzburg, and Augsburg in Bavaria region and Giessen and Kassel in Hesse region), previously designated as port of Rotterdam influence, and Hamburg has expanded also to Southern Austria, in Klagenfurt region, previously designated to road mode.

The importance of increasing cargo utilization factor to 80% had an important impact on transportation from Porto to Switzerland. A shift from the road-only path, considering the same route option available, but a 50% cargo utilization, to intermodal routes from the port of Genoa (Path 17) was noticed in every region of the country. Economies of scale were noticed in external costs related to the maritime transport that can affect the road mode due to its limited capacity. In Switzerland, comparing the lowest total external cost of transport chains in Scenario 1.1 and the lowest external cost of chain in Scenario 1.2, there was, on average, -14% reduction in costs with the chain configuration, and the highest reduction was noticed in Bellinzona, in Southern Switzerland, with -26% lower externalities (from 822 to 611 EUR/FEU).

Figure 6.6 presents the identification of the route with the least external cost in Scenario 2.2, in which it is considered additional intermodal routes and vehicle capacity is set to 80% of total cargo capacity. Table 6.5 shows the number of NUTS regions and their respective equivalent in area to each path preference shown in Scenario 2.2. Clearly, this is the case where alternative intermodal transport chain best performed, the area of influence of chains making use of maritime transport has increased in a more diverse range of ports and the road only transport mode decreased from 40% of total NUTS area in Scenario 1.1, considering fewer path option and a lower cargo utilization factor, to 24% in Scenario 2.2, allying environment-friendly transport chain in the extended transport network to larger cargo capacity utilization factor of 80% in vessel, trains and barges.

Table 6.5 – NUTS and areas in Scenario 2.2: full scope of intermodal routes (80% cargo capacity utilization)

Path ID	Description	#NUTS	%NUTS	#Area [1000 km^2]	%Area
1	Road	12	6%	530	24%
3	Containership (Rotterdam) + Road	27	14%	105	5%
13	Containership (Hamburg) + Road	39	21%	391	17%
14	Containership (Le Havre) + Road	36	19%	525	23%
15	Containership (Marseille) + Road	3	2%	85	4%
17	Containership (Setubal-Genova) + Road	18	10%	209	9%
18	Containership (Setubal-Genova-Salerno) + Road	7	4%	113	5%
19	Containership (Bilbao/Valencia) + Road	5	3%	51	2%
20	Containership (Liverpool) + Road	18	10%	128	6%
21	Containership (Tilbury) + Road	22	12%	102	5%
26	RoRo (Rotterdam)+ IWT(Basel) + Road	1	1%	3	0.1%
	Total	188	100%	2.242	100%

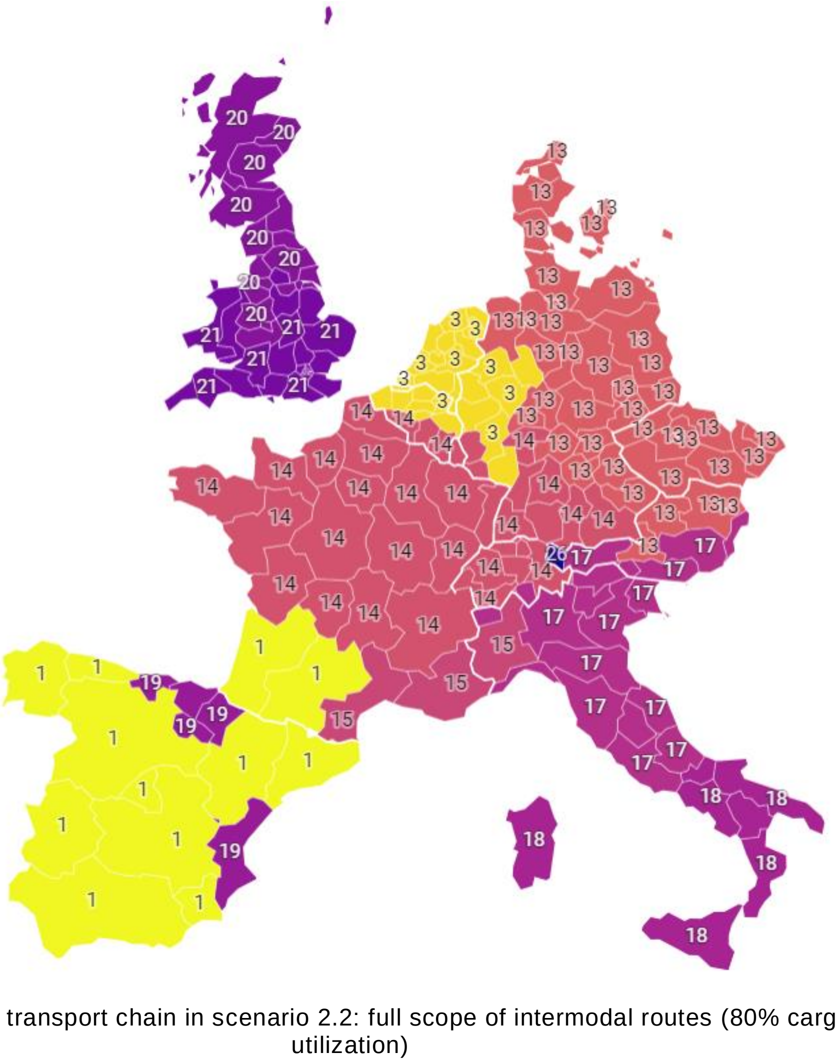


Figure 6.6 – Preferred transport chain in scenario 2.2: full scope of intermodal routes (80% cargo capacity utilization)

The enlargement of new containership lines is also noticed in Scenario 2.2, compared to Scenario 2.1, but in smaller intensity compared to the transition from Scenario 1.1 to 1.2. In the new routes' scenario, the port of Le Havre (Path 14) extended to Geneve (CH01) and Auvergne (FRK1), and port of Marseille to Languedoc-Roussillon (FRJ1), compared to Scenario 2.1.

Interestingly, in Austria, the minimum external cost to Bregenz, capital of Vorarlberg NUTS 2 region (AT34) occurs when making use of a RoRo vessel to the port of Rotterdam, transshipment in inland waterways to Basel, and then road modal to the destination (Path 26). Figure 6.7 presents external cost parcels that compose the total externalities related to transportation for each route possibility in Scenario 2.2. Despite a worse GHG emission performance, Air Pollution, Well-to-Tank, and Infrastructure costs demonstrated savings compared to transport chains through the port of Genoa, with rail transport to Basel (Paths 24 and 25).

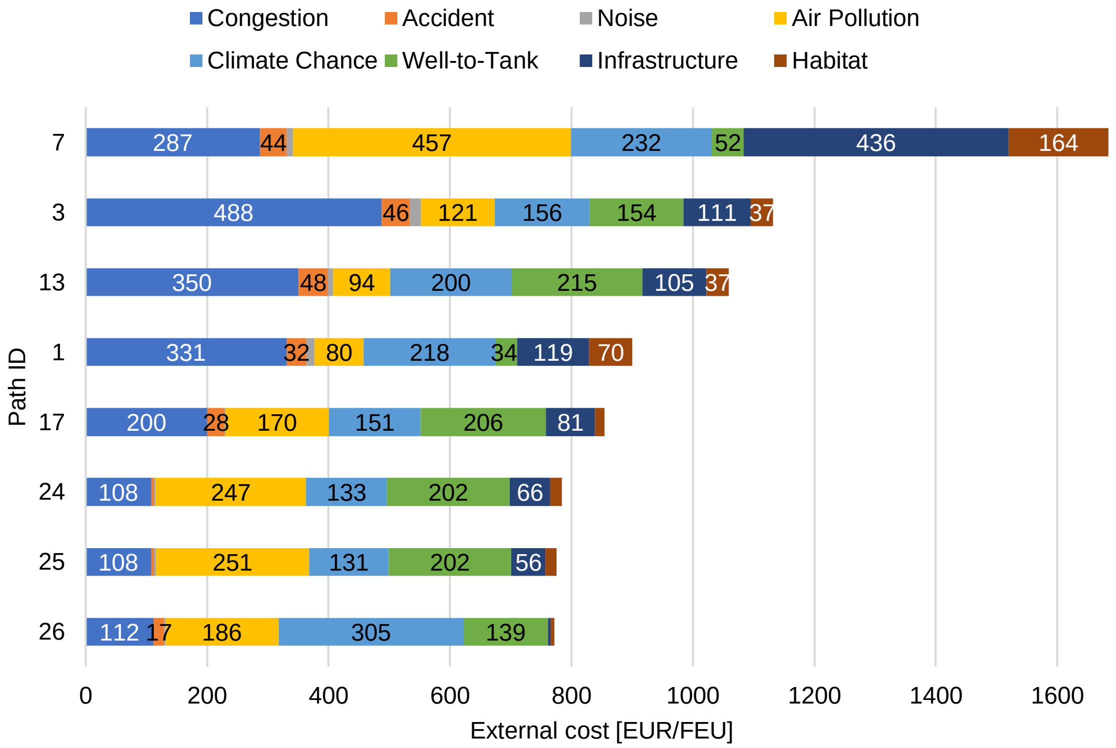


Figure 6.7 – Scenario 2.2: External costs in different paths to Bregenz (AT34)

To evaluate the effect of electric trains in all European railways covered by this study on the environmental impact of intermodal transport chains, Scenarios 2.3 and 2.4 make use of the complete set of only-road and intermodal routes from Porto, but the rail input parameter was set as electrical means of propulsion, with 50% and 80% cargo utilization, respectively. Figure 6.8 presents the chain preference map for Scenario 2.3 with regards to the route with minimum externalities for a 50% cargo capacity utilization in the train. Table 6.6 shows the number of NUTS 2 regions and its respective cover area corresponding to the preferable paths in Scenario 2.3. Comparing Scenario 2.3 to the case in which the same set of paths is used (full scope of intermodal transport chain) and the same cargo capacity utilization factor at 50% but considering only Diesel locomotives in all railways in the map (Scenario 2.1), the resulting transport chain preference map kept the same as can be seen in the Figure 6.3 and the Table 6.2. However, the external costs were reduced in this new condition since air pollutant externalities are reduced by using electric trains.

Table 6.6 – NUTS and areas in Scenario 2.3: electrical trains (50% cargo capacity utilization)

Path ID	Description	#NUTS	%NUTS	#Area [1000 km^2]	%Area
1	Road	20	11%	639	28%
3	Containership (Rotterdam)+Road	27	14%	109	5%
13	Containership (Hamburg)+Road	34	18%	345	15%
14	Containership (Le Havre) +Road	41	22%	539	24%
15	Containership (Marseille)+Road	2	1%	57	3%
17	Containership (Setubal-Genova) +Road	16	9%	202	9%
18	Containership (Setubal-Genova-Salerno) +Road	7	4%	113	5%
19	Containership (Bilbao) +Road	1	1%	7	0,3%
20	Containership (Liverpool)+Road	18	10%	128	6%
21	Containership (Tilbury)+Road	22	12%	102	5%
	Total	188	100%	2.242	100%

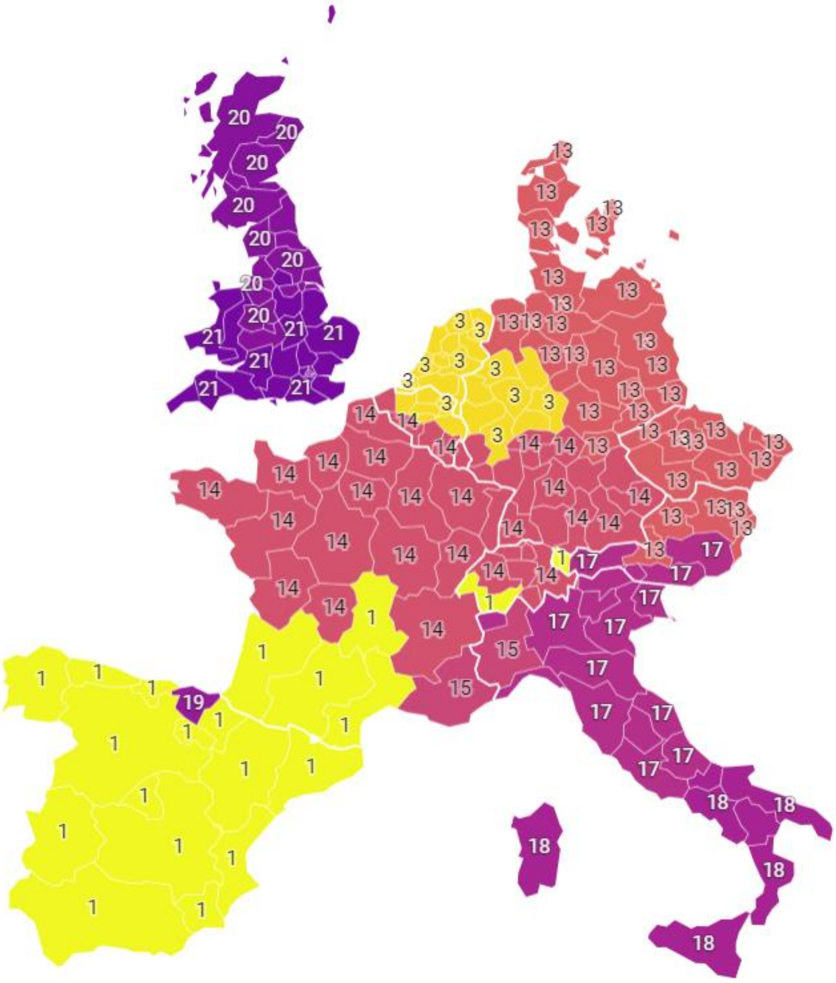


Figure 6.8 – Preferred transport chain in scenario 2.3: electrical trains (50% cargo capacity utilization)

Compared to Scenario 2.1, in which the set of routes and technical characteristics of other transport modes are the same, the use of an electric train at 50% capacity had no clear impact on the final chain preference map. Nevertheless, electric trains present zero Tank-to-Wheel emissions compared to Diesel locomotives, and externalities are exclusively related to the process of energy production and infrastructure costs.

Considering only the transport chain containing maritime transportation to Genoa, followed by railway transportation to Basel region before arriving in the destination by road (Path 25) in western France, Switzerland and southern Germany, Figure 6.9 presents the percentual reduction in the total external cost of Path 25, comparing Diesel and Electric traction, in regions covered by this route option. A geographic dependence can be noticed, in which reductions are higher close to Basel (-19%) with a lower impact to further regions (-13% in South Netherlands). On average, the total external cost has been reduced by -16%, due to -45% and -23% lower Air Pollution and Climate Change costs compared to Diesel locomotives. Even so, the external cost savings were limited by higher Infrastructure (11% higher) and Well-To-Tank costs (7% higher), associated with electric facilities and the energy production process, and the reduction was not sufficient to overcome advantages related to the cargo capacity of the containership, in further destinations, or only-road mode, in geographically closer destinations.

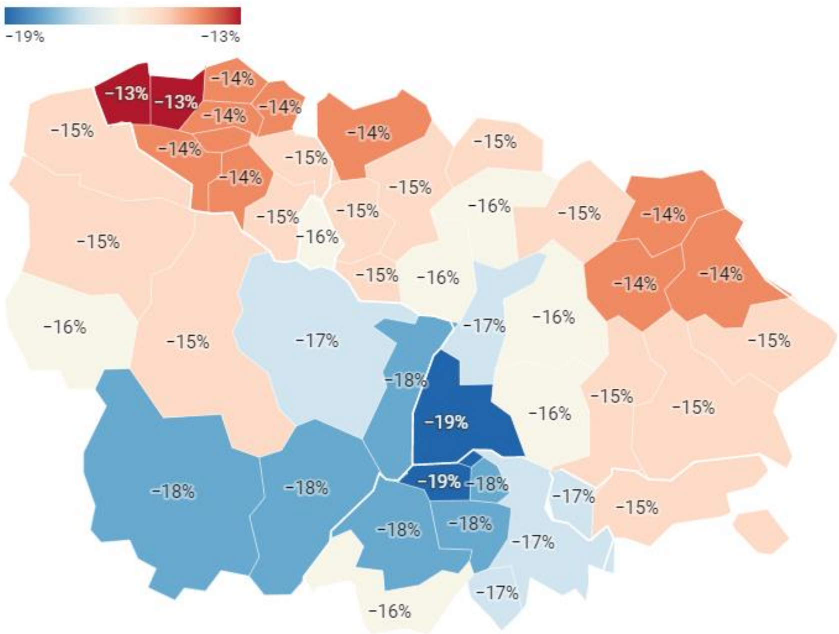


Figure 6.9 – External cost reduction caused by electric traction in the Genova-Basel segment of the intermodal chain

A similar analysis took place for the transport chain from rail terminal in Cacia, Portugal, to Mannheim (Path 7). The route contains a 3,000 km of railway traveled distance and it is responsible to serve 99 NUTS regions in Central Europe, i.e., northern France, the Netherlands, Luxembourg, Belgium, western Germany, Switzerland, Austria, and Czech Republic. When adopting electric traction, air pollutant and GHG emissions are abated during the Tank-to-Wheel (TTW) phases, then responsible for external costs reduction in Air Pollution and Climate Change parcels. On the other hand, the process of electric energy generation is responsible for significant emissions accounted in the Well-to-Tank external cost parcel. Additionally, electric trains are associated with sophisticated infrastructure and maintenance. Then, Table 6.7 presents a summary of some statistics about the percentual reductions or increments over the total external costs and some externalities by adopting electric traction in the geographical scope of Path 7.

Notably, the TTW air pollution emission was not reduced to zero due to the truck paths emissions. Even considering a significant increment in WTT external cost, the total external cost was reduced on average -34% by the new electric configuration. Figure 6.10 presents the percentual reductions in the total external costs per NUTS region, showing the highest reduction close to Mannheim intermodal rail terminal.

Table 6.7 – External cost percentage change by adopting electric trains compared to Diesel trains

Metric	Air Pollution	Climate Change	Well-to-Tank	Infrastructure	External Cost
Maximum	-99%	-95%	196%	11%	-38%
Minimum	-93%	-73%	249%	12%	-30%
Average	-96%	-85%	221%	12%	-34%

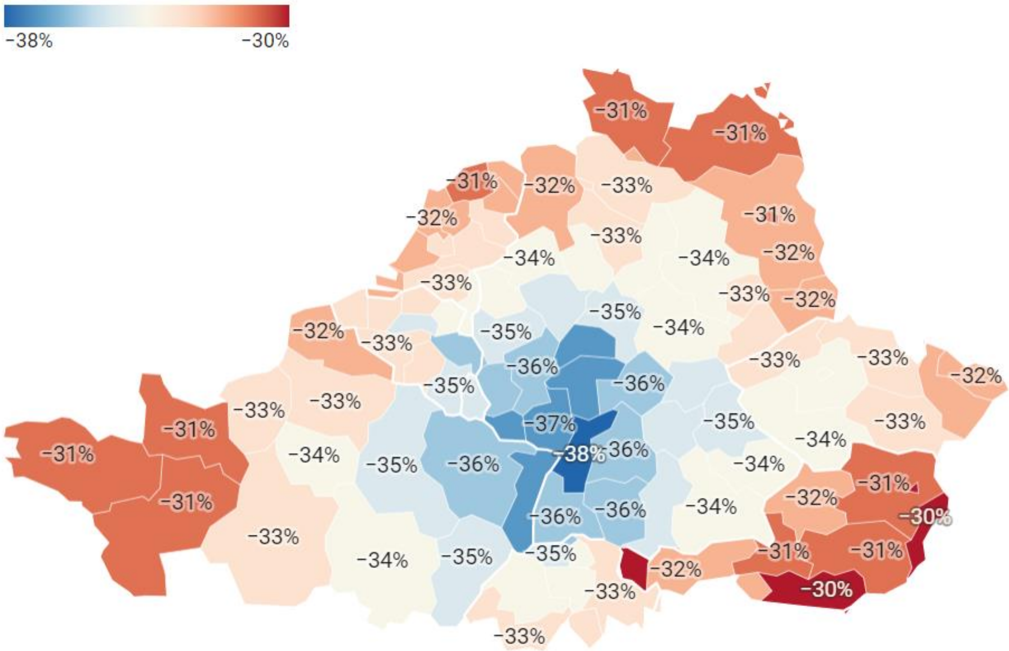


Figure 6.10 – External cost reduction caused by electric traction from Cacia to Mannheim railway terminal

Figure 6.11 shows the chain preference map for Scenario 2.4, in which electric traction is used at 80% of train cargo capacity. In this case, the combined maritime transport to Genoa and railway transport to Basel had the least human and environmental impact among other transport chains in several regions of Switzerland and Czech Republic. The reduction of costs per unit of cargo transported allied to the savings in the mentioned regions resulted in Path 25 preference in Switzerland regions below Basel (closer to the port of Genoa). Table 6.8 presents the number of NUTS regions and its respective area in each preferable path in Scenario 2.4. Here, a difference can be noticed by the introduction of path 25, including the railway transportation from port of Genoa to Basel region after maritime path in a container ship line.

Table 6.8 – NUTS and areas in Scenario 2.4: electrical trains (80% cargo capacity utilization)

Path ID	Description	#NUTS	%NUTS	#Area [1000 km^2]	%Area
1	Road	12	6%	530	24%
3	Containership (Rotterdam) + Road	27	14%	105	5%
13	Containership (Hamburg) + Road	39	21%	391	17%
14	Containership (Le Havre) + Road	32	17%	505	23%
15	Containership (Marseille) + Road	3	2%	85	4%
17	Containership (Setubal-Genova) + Road	18	10%	209	9%
18	Containership (Setubal-Genova-Salerno) + Road	7	4%	113	5%
19	Containership (Bilbao/Valencia) + Road	5	3%	51	2%
20	Containership (Liverpool) + Road	18	10%	128	6%
21	Containership (Tilbury) + Road	22	12%	102	5%
25	Containership (Genova) + Rail (Basel2) + Road	5	3%	23	1%
	Total	188	100%	2.242	100%

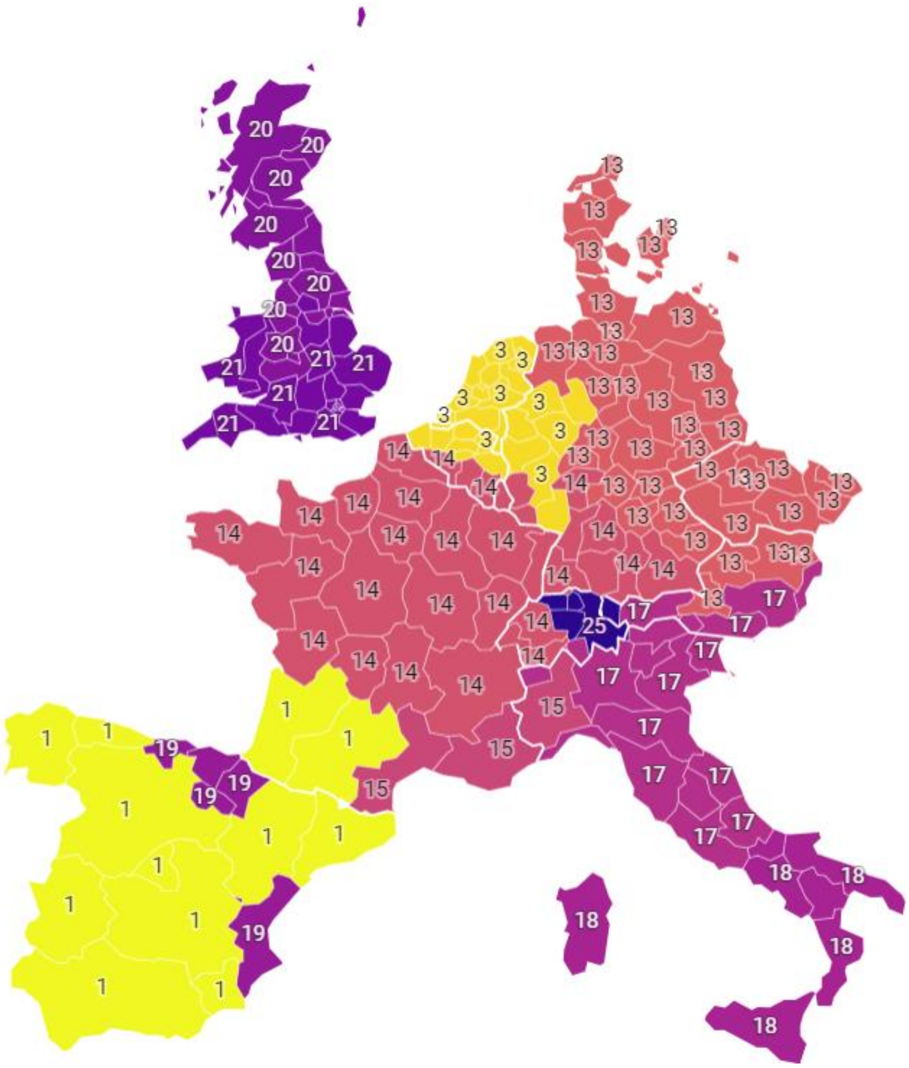


Figure 6.11 – Preferred transport chain in scenario 2.4: electrical trains (80% cargo capacity utilization)

For each region, the external cost and its parcels were compared in different pairs of scenarios. The chosen pair of scenarios were established in a way that the impact of a unique aspect of the transport chain was properly identified, keeping the other constant. The aspects here in focus are the introduction of new intermodal routes, increasing cargo capacity and the use of electric traction in railways. A comparative analysis of the impact of such aspects can also be done. Table 6.9 represents the average of the relative differences in the total external costs per unit of cargo in all regions in different pairs of scenarios.

Table 6.9 – Percentual savings by adopting intermodal chains, increasing cargo capacity, and use of electric traction in railways

Variable	From	To	Congestion	Accident	Noise	Air Pollution	Climate Change	WTT	Infra	Habitat	External cost
Intermodal chains at 50% capacity	1.1	2.1	-47%	-17%	-34%	-9%	10%	166%	-19%	4%	-15%
Intermodal chains at 80% capacity	1.2	2.2	-44%	-16%	-23%	-10%	7%	62%	1%	5%	-20%
Increase capacity in current chains	1.1	1.2	-21%	-33%	-57%	-19%	-22%	20%	-71%	-56%	-22%
Increase capacity in intermodal chains	2.1	2.2	-9%	-37%	-25%	-20%	-22%	-1%	-60%	-55%	-22%
Use of electric train at 80% capacity	2.2	2.4	-60%	-84%	-20%	95%	-44%	56%	325%	-1%	-10%

The table establishes the effectiveness of different strategies for reducing the environmental and human health impacts of transportation. The highest decrease in externalities is related to an increased cargo utilization factor, in which most externalities are reduced, resulting on average in a -22% reduction in the total external cost. Considering the current scope of transport chains, at 50% cargo utilization, the scenario has motivated a preference shift to maritime mode, associated with higher WTT emissions than other modes and, justifying 20% higher WTT cost. However, the full scope of intermodal chains was responsible for reducing -1% of WTT cost since the number of new maritime routes was lower. The remaining externalities, by adopting a higher capacity, have significantly decreased, and this aspect had a better performance in external cost savings.

Regarding the full scope of intermodal transport chains, the external cost reductions were also significant in Congestion, Accident and Noise, resulting in -15% and -20% lower total external costs at 50% and 80% cargo capacity, respectively. The fact of fewer only-road transportation was responsible for significant decrease in external cost parcels associated with truck operation. On the other hand, WTT emissions increased since ships' energy generation process is more polluted than in other modes. Slightly higher Climate Change and Habitat costs are noticed mostly because other externalities had a more penalizing weight on the total external cost, guiding its preference decision. The thesis provides a better solution considering overall externalities, but future studies are recommended for preference criteria guided by the minimization of GHG gases or another specific externality.

The effect of electric traction at 50% cargo capacity utilization was not sufficient to overcome maritime transport chains competitiveness even though externalities in rail transport chain had decreased (view Figure 6.9 and 6.10). For an increasing 80% cargo capacity utilization, the transport chain configuration was favorable to rail transport chains leading to -10% reduction on the total external cost. The percentages are basically related to the chain shift from containership route through Le Havre (path 14) to rail transport to Basel after passing by port of Genoa, in regions in Switzerland. The Air Pollution increment is not related to the emission reduction by adopting electric traction, but it is related to the worse air pollution emissions performance in the maritime path contained on the transport chain, i.e., the transport from Leixões to Genoa emitted more polluters than the maritime path to Le Havre, responsible for degrading the complete route that makes use of railway to Basel. Afterall, the total external cost in electrified railways is still lower than the maritime chain to Le Havre due to savings externalities related to the road mode.

The maps shown so far are related to the minimization of externalities to evaluate the environmental performance of transport chains using different combinations of modes of transport. The next subsection will present an economic study of the internalization of the external costs focusing on the changes of the route preference.

6.2 External Cost Internalization

Transportation cost traditionally consists of different cost parcels, composing the so-called internal cost. The transport cost here computed is based on specific costs of transportation – handling, tolls costs – computed using the software Intermodal Analyst (IA).

The set of transport chains available in Scenarios 1 and 2 have resulted in the maps shown in Figure 6.12 about the transport chain with the lowest internal cost. The unimodal road mode (Path 1) extends its preference to most regions, and regions geographically close to ports and intermodal terminals are considered suitable for transportation through intermodal transport chains. Different from Scenario 1, extra routes considered in Scenario 2 implied changes in specific regions, such as around the port of Le Havre (Path 14) in northern France, the port of Salerno (Path 18) in southern Italy, and the railway from Cacia (Path 7) in Darmstadt and Karlsruhe regions, in Germany. However, as stated in the previous section, long road distances are associated with more environmental and human impact and the monetarization of environmental impact may affect the map configuration. The general conclusion is that the extra intermodal routes in Scenario 2 have a limited capability for capturing more traffic when considering internal costs only.

The main objective of this thesis is to analyze how the introduction of the external cost in the traditional transportation cost impacts the chain preference above presented. For ding doing this, in each route, the external cost was algebraically summed to its corresponding internal cost, and the most competitive routes when considering also the environmental and economic aspects are obtained by identifying the route with the minimum total transportation cost. Then, new route preference maps can be drawn for each desired scenario.

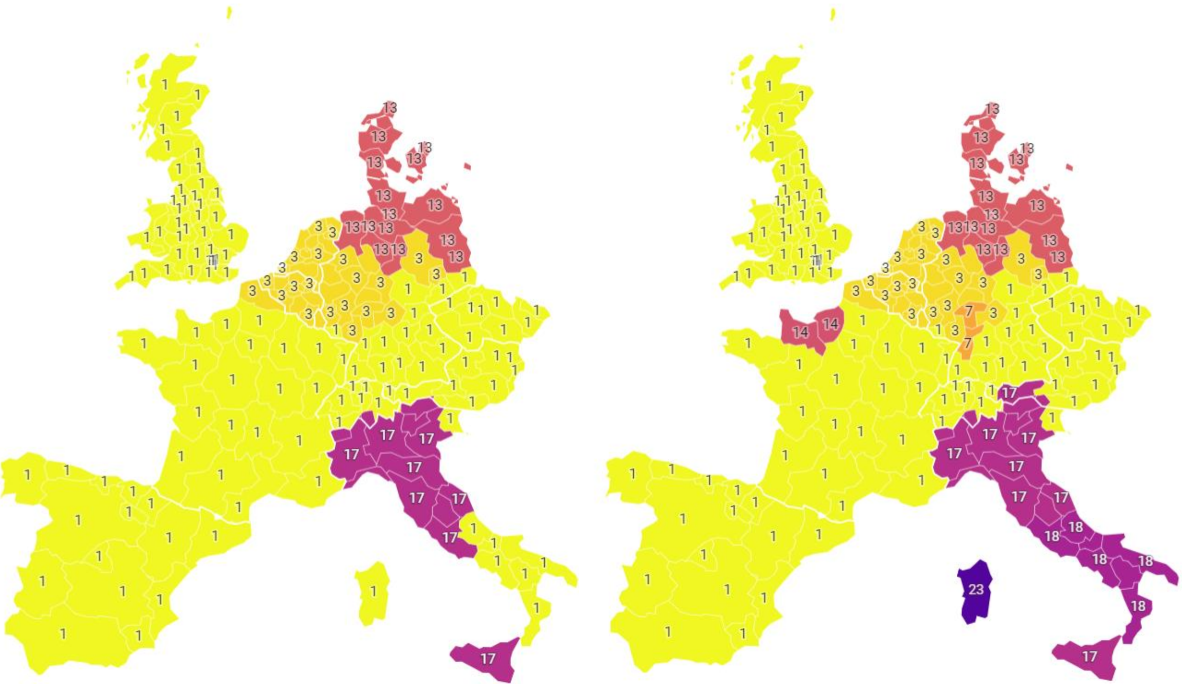


Figure 6.12 – Preferred transport chains regarding internal costs (Scenario 1 (left) and 2 (right))

Figure 6.13 presents the preference map, considering the Total cost, by using the current scope of transport chains with cargo occupation at 50% (Scenario 1.1) and 80% (Scenario 1.2). Some relevant modifications compared to the maps obtained when using the internal cost criterion (Figure 6.12) can be noticed due to the introduction of external costs in the cost structure, but still represents a modest configuration compared to the purely lowest external cost map in Figures 6.1 and 6.5 in Scenario 1.1 and 1.2, respectively. For instance, the preference for chains through the port of Rotterdam (Path 3) was limited to the Netherlands and a few regions in Germany, by accounting only for internal costs, but this area has expanded to northeastern France and most regions in Germany by accounting for externalities. This expansion is even larger considering vehicles at 80% capacity, in which also all regions in the Czech Republic adopted Path 3.

Although intermodal chains became more competitive, the environmental impact is limited by the order of magnitude of internal costs, representing most of the transportation cost. Considering the current scope of routes, on average, external costs represent 29% of the total transport cost when externalities are fully internalized. A more expensive carbon price (the carbon price used in these maps is 100 €/ton $CO_{2\text{-eq}}$) and higher marginal costs could affect the chain preference map based on the Total cost criterion in a way that this map can properly balance economic and environmental aspects.

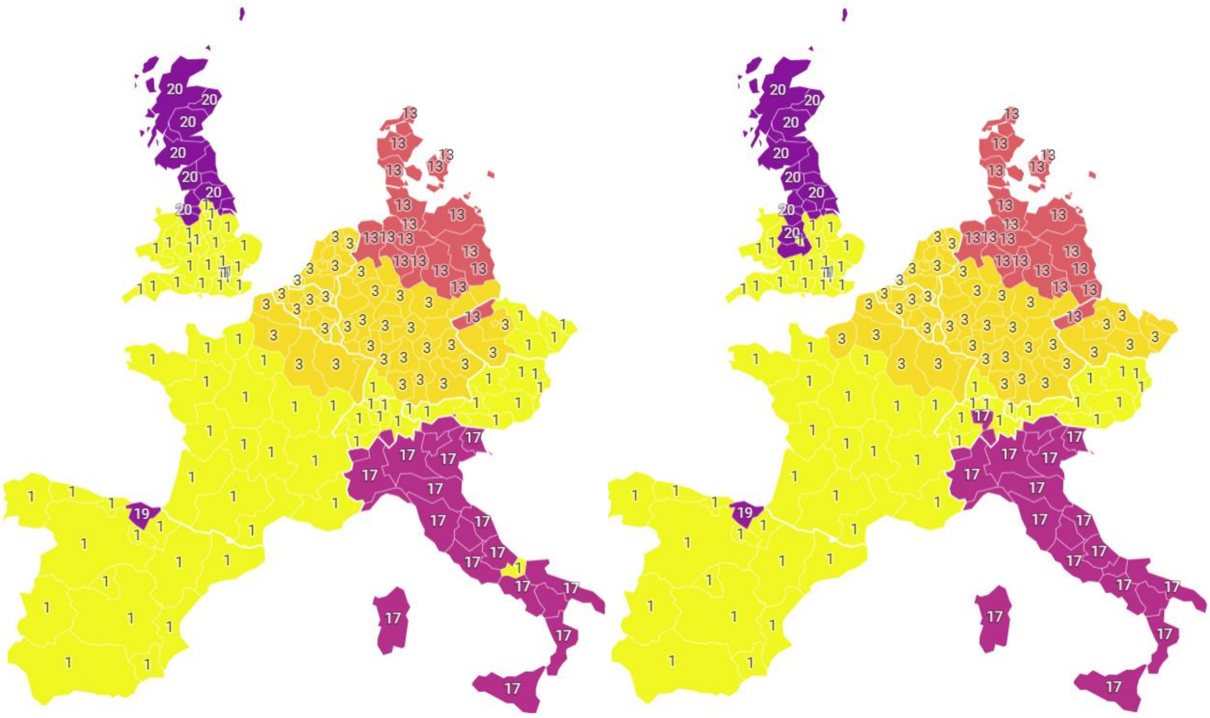


Figure 6.13 – Preferred transport chains regarding total transport cost (Scenario 1.1 (left) and 1.2 (right))

In the United Kingdom, the route preferences have also presented an important distinction compared to Figure 6.12. Route to port of Dover (Path 1) was replaced by port of Liverpool (Path 20) in the north of the island after considering new routes, in both cargo capacity utilizations. As can be analyzed from Figure 6.14, external costs form ferry route to the port of Dover (Path 1) increased the total transportation cost in a way that even the high internal cost associated with the containership to the port of Liverpool (Path 20) was compensated, resulting in the route shift noticed. Such increment of the external cost associated with RoRo vessel is caused by the high cargo capacity of the containership, added to the fact that installed power in the RoPax vessel is higher, emitting more air pollutants.

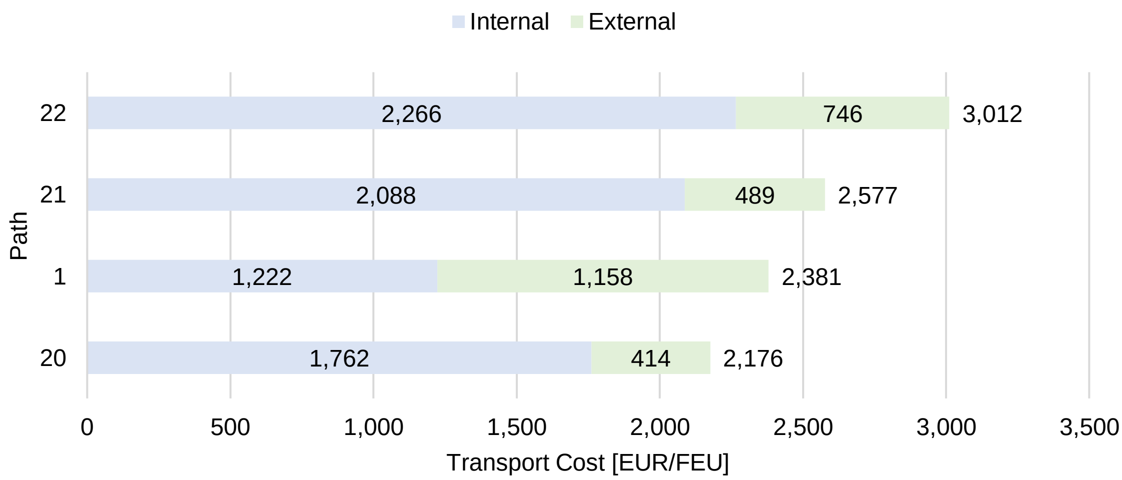


Figure 6.14 – Total transport cost per route to York (UKE2) in Scenario 2.2

Figure 6.15 shows the route preference map regarding Total cost for the full scope of intermodal transport chains at 50% and 80% cargo capacity utilization. A similar map was obtained when compared to Figure 6.12, but in this case, additional routes are considered in the route possibilities and some of them have performed better than the previous set. Regions concerning the use of ports of Le Havre, Salerno, and Marseille can now be seen on the map. Again, a modest approximation of the total transport cost map to the map based on the external cost is noticed, for example, the restricted area of port of Le Havre before dominated France and Germany region in Figures 6.3 and 6.6.

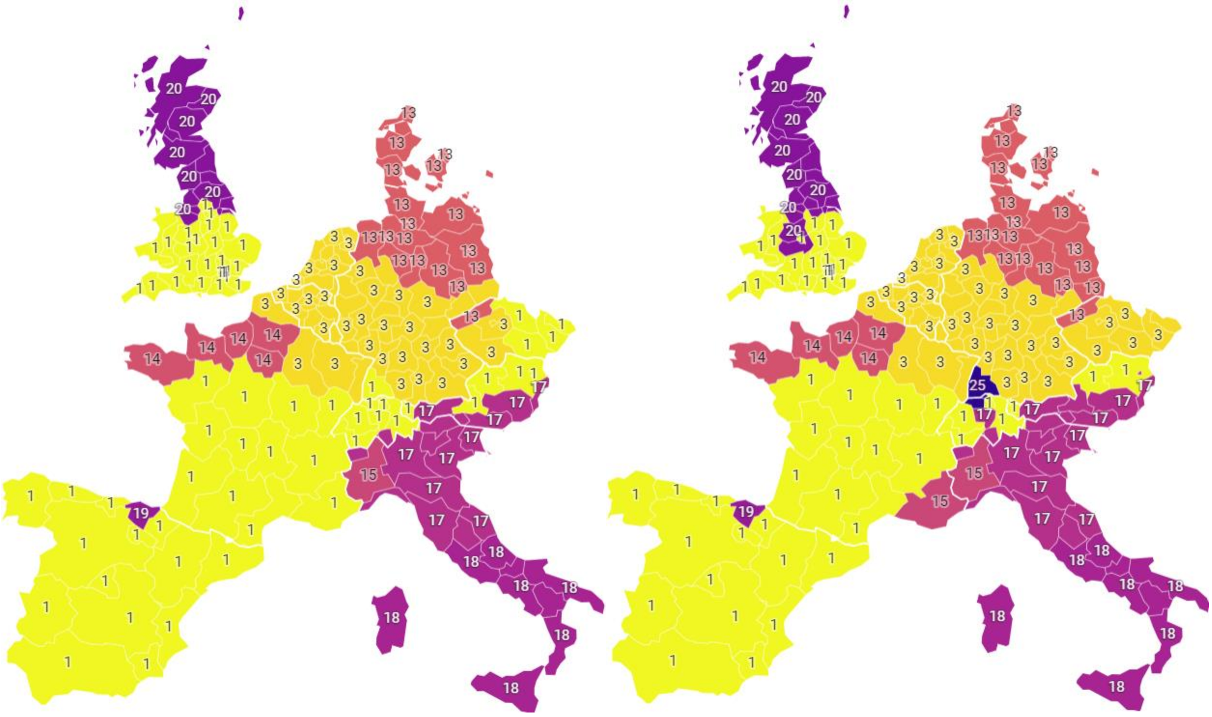


Figure 6.15 – Preferred transport chain regarding total transport cost (Scenario 2.1 (left) and 2.2 (right))

A preference change can also be noticed by the introduction of routes that performed better regarding externalities, but also regarding internal costs. For instance, the current routes to the longest road distance region in Austria – Eisenstadt (AT11) – are only-road (Path 1), the port of Rotterdam (Path 3), and the port of Hamburg (Path 13), but the full scope of intermodal routes includes also Cacia railway terminal (Path 7) and the port of Genoa (Path 17). At 80% cargo capacity, total transport costs per unit of cargo are shown in Figure 6.16. Considering the actual set of paths, Path 1 is the most competitive route by internal and total costs criteria, although Path 13 presents the lowest environmental impact in this scenario. However, when the full scope of routes is considered in Scenario 2, the external cost in the route through port of Genoa (Path 17) compensates the small difference in internal costs between the only-road transport (Path 1), resulting in the path 17 preference with a better environmental and internal cost performance than in Scenario 1, in which path 3 was chosen.

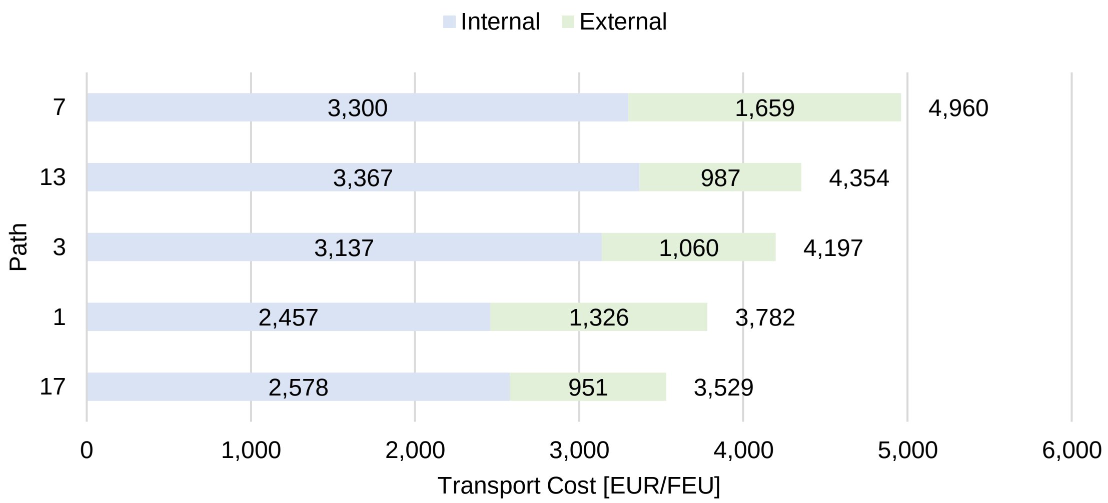


Figure 6.16 – Total transport cost per route to Eisenstadt (AT11) in Scenario 2.2

Considering Scenario 2.2, in which the full scope of the intermodal routes is carried out by vessels and trains at 80% cargo capacity, regions on the border of Germany and Switzerland are served by railway lines through Basel, after arrival in the port of Genoa (Path 25). However, in this region, the external cost of the route through the port of Le Havre (Path 14) is 486 EUR/FEU, -30% lower than the one of the chosen Path 25 (681 EUR/FEU). On the other hand, the route from the French port presents a 37% higher internal cost than the combination of SSS and rail transport mode (2,938 EUR/FEU compared to 2,152 EUR/FEU). Table 6.10 presents the rank of Path 25 with regards to internal and external costs, separately, and Figure 6.17 shows the total transportation cost per route to Freiburg (DE13). Even if the route from Genoa has not the lowest internal or external cost, the combined effect of both costs led to railway mode preference, able to balance a reasonable environmental and economic performance of transportation.

Table 6.10 – Railway lines cost comparative performance to Freiburg (DE13) in Scenario 2.2

Path Description	Path	External cost	Internal cost
Containership (Le Havre) + Road	14	1º	10º
Containership (Genoa)+Rail (Basel2) + Road	25	3º	2º
Road	1	9º	1º

Paths 11 and 12 have approximately 50% higher total transport cost than the average total cost of all route possibilities to Freiburg (DE13) in Scenario 2.2. Part of the full scope of intermodal routes scenario at 50% cargo capacity (Scenario 2.2), paths 11 and 12 connecting Porto to Freiburg (DE13) presented the worse total cost of transportation performance, because of the highest internal and external costs. Figure 6.18 shows external cost parcels in the 5th worst paths in external cost performance. Firstly, Path 11 is composed of a SSS service from port of Leixões to port of Hamburg, followed by road mode to the destination. The RoRo ship travels 1,398 nm (2,589 km) at sea and its associated capacity is 217 FEUs (almost one fourth of containership capacity used in path 2 to Rotterdam), and the installed power is considerably higher, implying in higher fuel consumptions and emissions. From the port of Hamburg, the destination is in one of the furthest regions from the port with 750 km road distance, approximately. The high fuel consumption in maritime mode allied to long road distance resulted in considerably increments in Climate Change and Air Pollution costs. In the intermodal Path 12, the maritime path from port of Leixões to port of Hamburg is also carried out by the same RoRo vessel. The transshipment to the railway corridor of Wurzburg did not provide savings enough to compensate for the direct road transport from Hamburg to the destination. For this reason, the GHG and air pollutant emissions were also responsible for the degradation of route 12, and the total external costs were comparable to the worst path 11. Besides externalities, internal costs associated to these routes are disproportional in RoRo lines, resulting in high total transport costs.

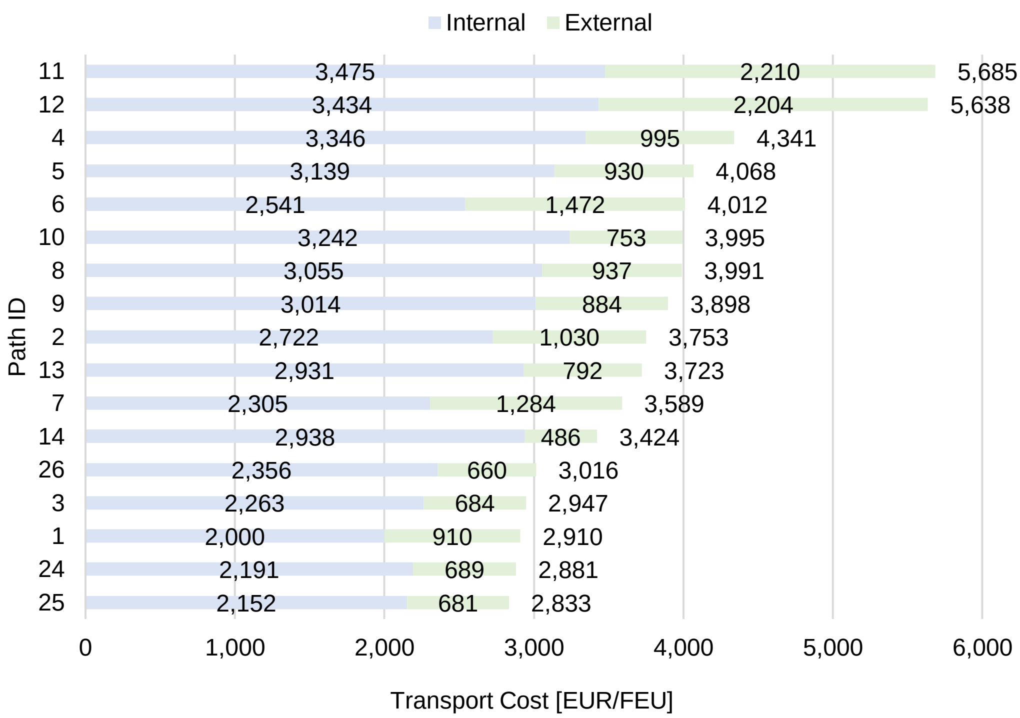


Figure 6.17 – Total transport cost per route to Freiburg (DE13) in Scenario 2.2

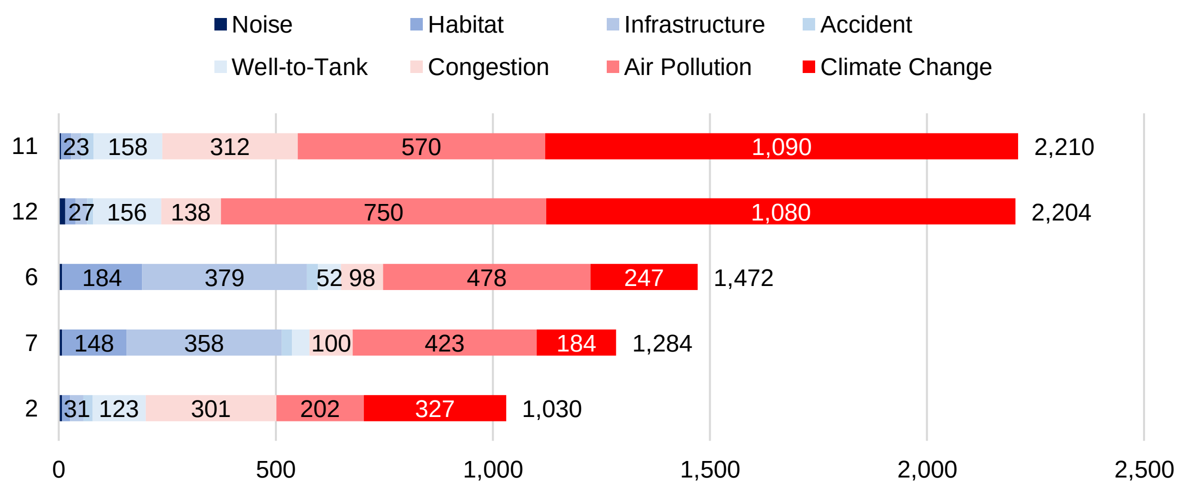


Figure 6.18 – External cost parcels for the 5th worst paths to Freiburg (DE13)

Figure 6.19 indicates the preferable route option based on the minimum total transport cost, considering electric trains on railways at 50% (Scenario 2.3) and 80% (Scenario 2.4) cargo utilization factors. Differently from the external cost preference map, considering a 50% cargo occupation, the map was able to present a different region preference compared to Scenario 2.1, with a railway route in Basel. As previously mentioned, the balance between internal and external costs of railway mode was responsible for the change from the preference map based on the external cost to total transport cost.

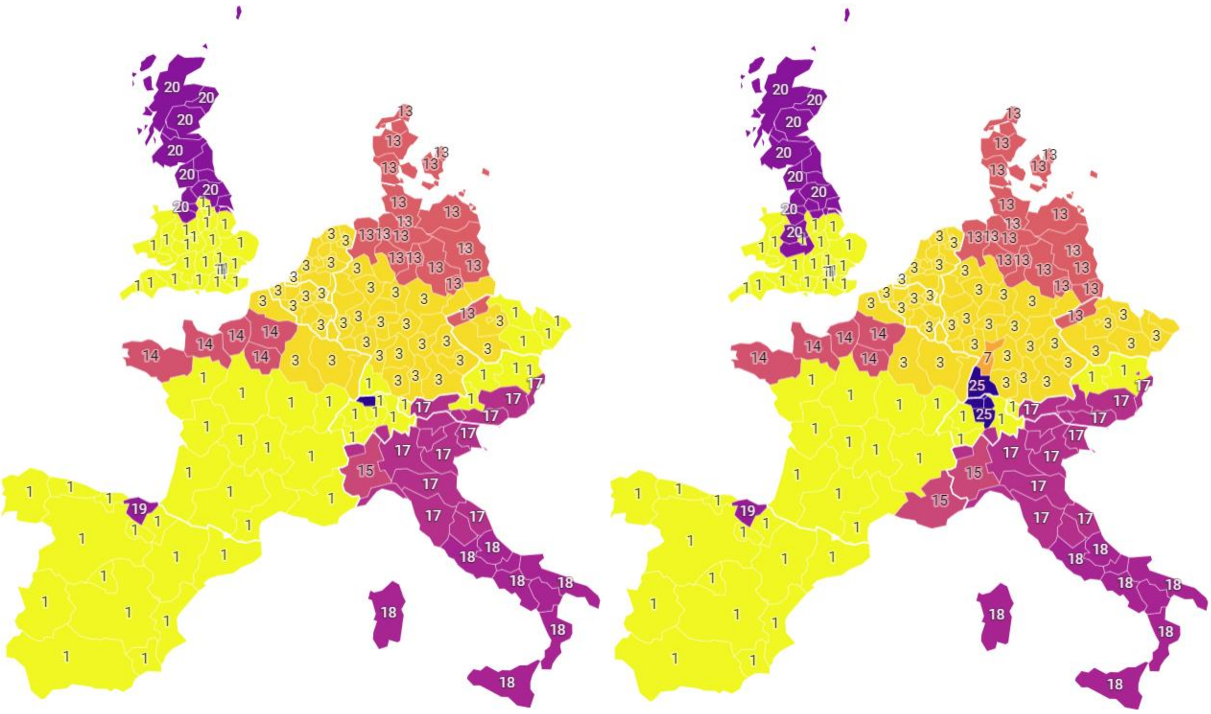


Figure 6.19 - Scenario 2: Electrical train at 50% (left) and at 80% (right) cargo capacity

The direct transportation through the Atlantic railway corridor from Entroncamento railway terminal, in Portugal, to Mannheim railway terminal, in Germany (Path 6), is not considered an optimum solution in terms of environmental and economic performance in any set of maps previously presented. The railway path is part of chains to northern France, Belgium, the Netherlands, Luxemburg, and Germany by road mode. The total external costs in path 6 are composed by a constant railway external cost from Entroncamento to Mannheim, constant for all destinations, and the end-door transport is carried out by road, which varies in accordance with the destinations. The same modal split is considered in the railway transport from Cacia, in Portugal, to Mannheim, following by road to the destination, but in this case, it extends also to Austria, Czech Republic and Switzerland.

Figure 6.20 presents the constant railway external cost parcels in both paths 6 and 7. Even if Air Pollution and Climate Change are not generated in electric traction, great part of external cost degradation in the railway corridor is related to high infrastructure cost of electric traction, increasing Well-to-Tank emission and habitat damage cost. According to map in Figure 6.21, the road external cost decreases as the destination is closer to the Mannheim terminal (DE12). In this region, when considered train at 80% capacity (Figure 6.19 - right), the region with the lowest road external cost is served by path 7 (lowest total transport cost).

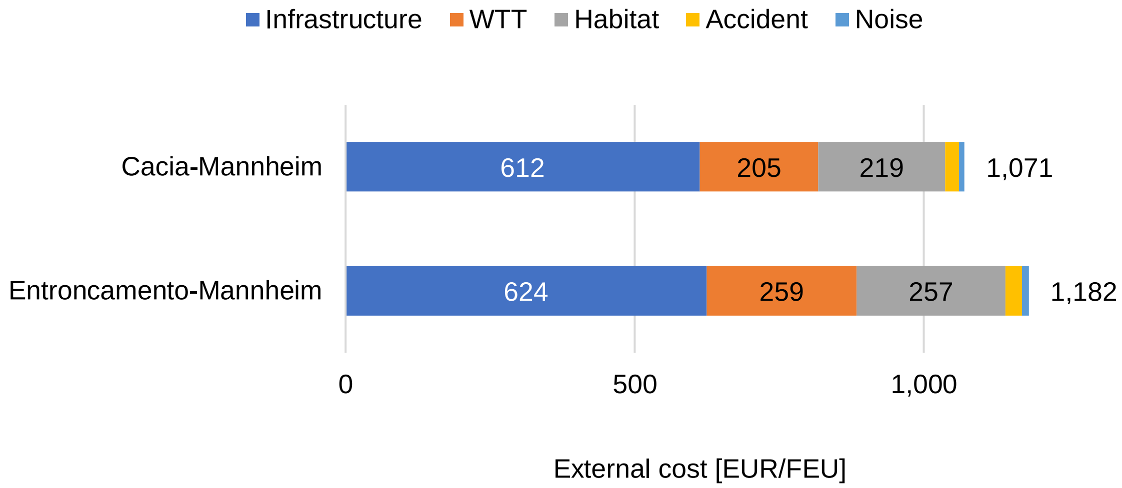


Figure 6.20 – Railway external costs in Paths 6 (Entroncamento) and 7 (Cacia)

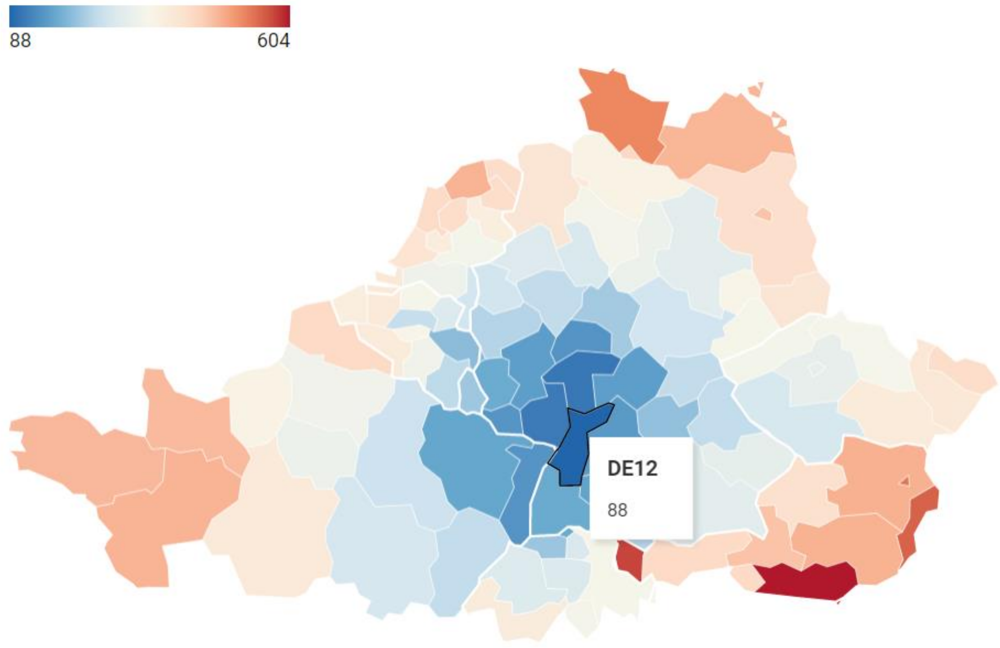


Figure 6.21 – Road external cost in €/FEU from Mannheim terminal (DE12)

Besides the railway from Cacia (Path 7) in Scenario 2.4 (right Figure 6.19), the preference for path 25 covers two extra regions in Switzerland compared to Scenario 2.2 (right Figure 6.15), based on the total transport cost using Diesel locomotives, also at 80% capacity. Figure 6.22 presents a comparison between path 25 connecting Porto to Zurich, comparing Diesel (Scenario 2.2) and electric traction (Scenario 2.4). The same internal cost is associated to Path 25 in both conditions and then, the internalization of external cost is responsible for increasing competitiveness of electric traction. Of course, externalities related only to road mode and distance (Congestion, Noise, Infrastructure, Accident and Habitat costs) are the same in both cases, but electric air pollution corresponds to 56% of Diesel pollution in whole transport chain and GHG emission is 75% of emissions using Diesel, balancing the increment of 7% in electric locomotives WTT cost.

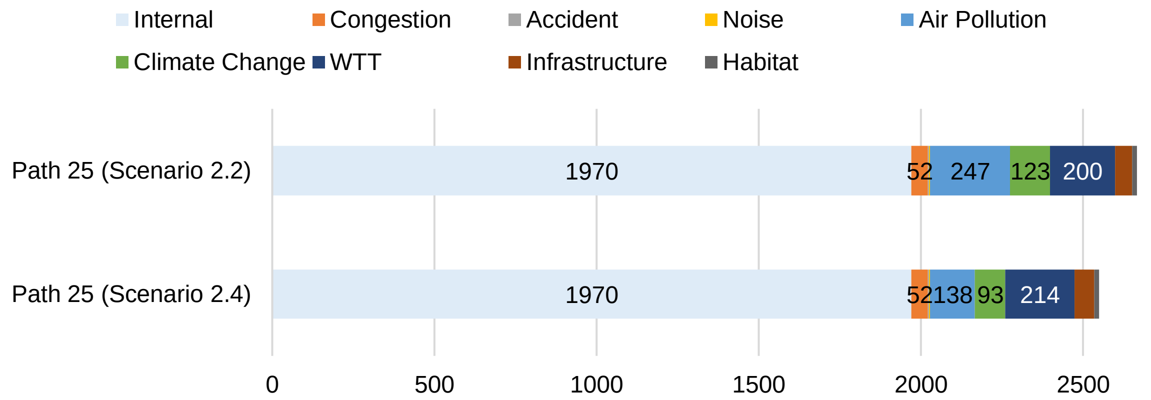


Figure 6.22 – External cost parcels in path 25 to Zurich (CH04) using Diesel and electric locomotive

Generally, Table 6.11 summarizes the number of NUTS regions in which the transport chain changed from the least internal cost map to the external cost internalization map, highlighting the mode of transport and intermodal terminal involved in this change. It is possible to conclude that more than 85% of modal shifts in all scenarios tested concern the adoption of water-borne transportation instead of only-road mode. Short-Sea-Shipping routes in Europe became more competitive when externalities related to transportation are considered as included in the transportation cost (internalization) rather than when just internal transportation costs are considered. Even though WTT costs have strong influence in ship's total external cost, some externalities related to road mode are considered negligible in ships, such as Accident, Noise and Congestion, penalizing chains with long road distances. Furthermore, the remaining modal shifts were also associated with a preference for maritime transportation, in which just the port or set of ports are modified. These last shifts are caused by specific vehicle characteristics associated with each route - such as the vessel's capacity and installed power, train's length –, but also terminal-specific costs, responsible for lower internal costs.

Notably, considering the full scope of routes (Scenario 2) was responsible for the highest number of preference changes due to the environmental advantages presented by intermodal routes, most of them still are not used. A broader range of route possibilities, comprising intermodal paths in different ports of call, presented a reduction in external costs and a consequent increase in competitiveness of other modes of transportation. Summed to a higher cargo utilization factor, the number of modal shifts goes up to 33% of all regions considered. More route preference shifts could be reached if external costs did not have only a 29% participation in the total cost of transportation.

Table 6.11 – Number of NUTS 2 regions affected by external cost internalization per scenario

Path description		**Scenario**					
Before internalization	**After internalization**	**1.1**	**1.2**	**2.1**	**2.2**	**2.3**	**2.4**
Only-road	Containership (Rotterdam)	20	24	18	21	18	21
Only-road	Containership (Genova)+Rail (Basel2)	0	0	0	2	1	4
Only-road	Containership (Hamburg)	1	2	1	2	1	2
Only-road	Containership (Le Havre)	0	0	3	3	3	3
Only-road	Containership (Marseille)	0	0	0	1	0	1
Only-road	Containership (Setubal-Genova)	7	9	4	7	4	6
Only-road	Containership (Bilbao)	1	1	1	1	1	1
Only-road	Containership (Liverpool)	14	18	14	18	14	18
Rail (Cacia)	Containership (Rotterdam)	0	0	2	2	2	1
Containership (Rotterdam)	Containership (Hamburg)	2	2	2	2	2	2
Containership (Setubal-Genova)	Containership (Marseille)	0	0	1	1	1	1
Containership (Setubal-Genova)	Containership (Setubal-Genova-Salerno)	0	0	1	1	1	1
RoRo (Livorno)	Containership (Setubal-Genova-Salerno)	0	0	1	1	1	1
	Sum	45	56	48	62	49	62
	%Regions	24%	30%	26%	33%	26%	33%

7. CONCLUSIONS

The environmental and human health impacts of a transportation network from Porto to major European commercial partners of Portugal were assessed by the new version of the software Sustainability Analyst (SA). The Portuguese commercial trade in Europe was evaluated using existing transport chains and new intermodal transport chains from different perspectives, not only focusing on the traditional components of transportation cost but considering also externalities related to the transportation. The competitiveness of the new scope of transport chains through ports on the West Mediterranean, the Atlantic railway corridor and new port of calls in the North Sea was evaluated based on the analysis of similarities and differences between maps containing the preferable routes regarding internal, external, and total transportation costs.

Before going through the main conclusions, some technical remarks about the software's functioning must be mentioned. Modifications to the software were carried out in a way to allow the correct application of the mathematical model in different numbers of route possibilities for each pair O/D. Additionally, each route is now related to a specific vehicle's technical characteristics, being possible for instance to use the same route with a different ship's main particulars or train's length without having to create a new path. Stronger interconnectivity between the internal cost software (Intermodal Analyst, IA), and the Sustainability Analyst was created by introducing additional IA results and computing total transportation costs. This way, the time of data post-processing using other tools is reduced since the route with the lowest costs is already internally obtained for each pair O/D. Externalities related to habitat degradation due to transport activity were included in this SA version, comprising thus a broader range of external costs parcels following the guidance of the Handbook of External Cost of Transport (CE Delft, 2019). To keep the consistence of emissions mathematical model, railway emissions cover fuel consumption dependency with locomotive installed power and trains speed, coping with Diesel locomotives EU emission standards.

Some advantages can be found in the implemented mathematical model for computing exhaust gas emissions when compared to existing online calculators. The degree of detail in the vehicle characterization in every mode of transport is considerable compared to other tools, for example, Mesoscopic, ARTEMIS, and ETW models, in which emissions do not vary for important parameters in rail and road modes (Heinold A., 2020). Usually, these tools compute pollutant emissions for specific modes of transportation, and rarely cover the full scope of intermodal chains, making it difficult to help the decision process considering a vast number of route possibilities. Besides this fact, they are restricted to pollutant estimations and do not cover estimations of other major externalities related to transportation. As demonstrated in Chapter 6, in some regions, the route preference is strongly sensitive to some externalities, such as Well-To-Tank and Congestion, leading to divergent decisions regarding the most sustainable route. In fact, accounting for a broad number of variables is necessary to properly represent the current state of development of the transport network and possible transport chains.

7.1 Main conclusions

Regarding the results about preferable routes regarding the minimum external cost route option, some conclusions can be obtained:

- Short-Sea-Shipping (SSS) from Portugal to destinations in Central and Western Europe had at least 40% lower external costs by the adoption of transport chains through Western European ports, such as ports of Hamburg and Rotterdam. The percentual reduction is even higher on regions close to the port areas and considering vessels with a higher cargo capacity utilization.
- The increasing competitiveness of the full scope of intermodal transport chains, due to about 15% lower external costs, has allowed 7% higher number of NUTS2 regions served preferably by SSS services (at 50% cargo capacity utilization).
- Only 3 external costs are related to SSS services compared to 8 parcels in road mode, but Well-To-Tank (WTT) emissions has a major impact on maritime services. WTT cost is, on average, 35% of maritime transport external cost, considering 50% cargo utilization, and 33%, considering 80% utilization. For this reason, economies of scale indicate a strategy for increasing SSS competitiveness so the cost per unit of cargo is reduced.
- Inland waterway transportation (IWT) presents advantages in Air Pollution, Well-to-Tank, and Infrastructure costs leading to a transport chain preference that implies using the RoRo ship to port of Rotterdam, followed by IWT to Basel (path 26), in the full scope of intermodal routes at 80% cargo capacity (Figure 6.6). However, IWT chains 25 and 26 did not perform well in most cases due to the high savings allowed by container ships in comparison to RoRo vessels, when associate to IWT.
- Electric trains affected the chain preference configuration considering high cargo utilization factors. Even though external costs using electric traction were reduced by 16% due to zero emissions, savings were not sufficient to overcome maritime transport advantages.
- The road-only mode option is environmentally justified in relatively short road distance to the destination, depending on the other modes' technical characteristics. Routes through intermodal terminals, such as ports and railway terminals, are not justified when the destination is geographically close to Portugal, which would include additional road distances from the terminal to the destination in a way that environmental performance is penalized. This was the case in certain regions in Spain, distant to Valencia and Bilbao Ports, and France, depending on the vessel's characteristics.

Regarding the effects of the fully internalization of external cost in the transportation cost in a way to evaluate the route preference comprising environmental externalities and internal costs of transportation, the analysis of the maps showing route preference led to the conclusions below stated:

- The total transport cost criteria, accounting with the fully internalization of external costs, presented an increasing competitiveness of SSS transport preference. Compared to preferred chains regarding the least internal cost, transport chain preferences changed from road-only transport mode to SSS services in 22% of NUTS 2 (44 out of 188 regions), considering 50% cargo capacity utilization and Diesel locomotives, and 30% of NUTS 2 (56 out of 188 regions), considering vehicles at 80% cargo capacity utilization and electric locomotives.

- Considering the full scope of intermodal transport chains, the number of NUTS 2 regions that changed its preference, regarding the least total transport cost, compared to the current scope of intermodal chains was 10% (19 out of 188 regions), at 50% cargo capacity, and 13% (24 out of 188 regions), at 80% cargo capacity. Most of preference changes was related to the adoption of new chains through ports of Le Havre, Marseille, and Genoa, nowadays commonly used by shippers from port of Leixões.
- Even though transport chain preference was impacted by the external cost internalization, map preferences regarding the least total transport cost resulted in a close similarity with routes options in those maps regarding internal cost minimization, not reflecting the external costs advantages of some routes presented in maps regarding external cost. This fact is related to the order of magnitude of external costs, comprising on average only 29% of total internalized transport cost.
- In regions close to rail terminals, intermodal routes comprising maritime and railway paths were preferable concerning total cost, even if it is not the option with the lowest externalities. The balance between internal and external costs for a decreasing total cost is even noticed in further regions in Switzerland and Germany when considering electric traction trains.
- Accounting only for internal transport costs, the road-only mode is the most competitive route due to fewer costs in comparison to chains involving the use of intermodal terminals. In this context, intermodal chains are preferable only in regions with good connections between different transport modes, such as in the Netherlands and northern Germany.

Some limitations regarding the methodology here applied can be mentioned, mostly associated to the emission estimation methos. Emissions estimation based on emission factors and monetarization of externalities using marginal costs are basic steps for these external cost estimations. However, numerous uncertainties concerning emission factor data application for different vehicle types, the accuracy factors, accuracy of ship AIS data, low steam emissions and others. Regarding the external cost factors, external costs still are not fully representative of externalities, divergent policy decisions may result in this process (Merchan, et al., 2019). Indeed, intermodal transport chain competitiveness was impacted by varying vehicle technical characteristics.

Additionally, for the sake of the real impact of results here presented cooperation between transport stakeholders to reduce externalities must be intensified (Zhang, et al., 2022). Collaborative planning in Intermodal transportation requires active cooperation among carriers to achieve emission reductions in an effective way. However, the route decision-making process should also take in consideration externalities of the transport sector to meet climate change goals established by international and local governmental organizations and returning to the society negative impacts of transport activity.

7.2 Future developments

Extensions of the SA software can be further developed to assess the impact of developing regulations and new methodologies. Among them, the life cycle assessment (LCA) methods are commonly found in the literature for assessing the cost of Well-to-Tank and Tank-to-Wheel emissions, offering reliable numerical estimations of emissions. Methodologies such as LCA would give a broader perspective on emissions in transport activity over vehicle lifetime span.

Furthermore, the effectiveness of new regulations for meeting the EU Green Deal goals, as described on the ‘Fit for 55’ packages, can be assessed by this computational tool. The application of the emission estimation numerical method focused on the transportation chains in Europe can be used to compute carbon savings by varying carbon prices, introduced by ETS, and new fuel regulations.

In this thesis, Well-to-Tank emissions are only considered monetized by external costs, but the mass of air pollutants produced in this phase are not explicitly computed. Besides this fact, for a smaller scope of scenarios an analysis could be carried out by minimization of air pollutants and GHG emission separately to avoid carbon leakage to countries with local more competitive marginal external costs.

Additionally, the results of external costs here computed in different European countries could be applied to evaluate the degree of internalization of European market-based measures. Taxations over environmental performance and related human health issues in different modes of transportation can be compared to the monetize externalities to give a perspective of how these measures perform in compensating negative impacts of transportation to the society.

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