BRNO UNIVERSITY OF TECHNOLOGY

VYSOKÉ UČENÍ TECHNICKÉ V BRNĚ

FACULTY OF MECHANICAL ENGINEERING

FAKULTA STROJNÍHO INŽENÝRSTVÍ

INSTITUTE OF PROCESS ENGINEERING

ÚSTAV PROCESNÍHO INŽENÝRSTVÍ

MINIMISING EMISSION FOOTPRINTS IN CIRCULAR ECONOMY BY PROCESS INTEGRATION

MINIMALIZACE EMISNÍCH STOP V OBĚHOVÉ EKONOMICE METODOU INTEGRACE PROCESŮ

DOCTORAL THESIS
DIZERTAČNÍ PRÁCE

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BRNO 2019

KEYWORDS:

Emission Footprints, Process Integration Methodology Extension, Circular Economy, Waste Management, Reduction of Transportation Emissions

KLÍČOVÁ SLOVA

Emisní stopy, Rozšířená metoda integrace procesů, Oběhová Ekonomika, Management odpadů, Snížení dopravních emisí

CITATION

Fan, Yee Van. Minimising Emission Footprints in Circular Economy by Process Integration: Transportation and Waste Management. PhD thesis, Brno: the Brno University of Technology, Faculty of Mechanical Engineering, Institute of Process Engineering, 2019. Supervisor Jiří Jaromír Klemeš.

Declaration

I declare that I am the author of this doctoral thesis. It has been prepared under the guidance of my supervisors. The reported results are original research which developed based on my knowledge gained during PhD study and consultation with experts. I have quoted all the sources including own publications. The related references are provided at the end of this thesis

Brno: Yee Van FAN

Abstract

This thesis presents methodologies that have been developed to reduce emission footprints in the context of a transition to a Circular Economy through the application of a Process Integration approach to analysis and design, while also addressing challenges which have previously prevented practical implementation. Environmental sustainability, which is frequently indicated by low emissions and waste footprints, plays a critical role in facilitating the transition towards a Circular Economy. Three methodologies which are based on the breakeven concept and the extension of Pinch Analysis and P-Graph frameworks are proposed. The applicability of these methodologies is demonstrated by six case studies focused on transportation and waste management. My contributions to the field include:

(i) A novel breakeven based decision-making tool, with parallels to the classical phase diagram that aids rapid decision-making on the processes (e.g. selection of transport mode for a given distance and load) with the lowest environmental burden.

(ii) An emissions accounting system which aggregates GHG, SO_x, PM and NO_2 as a Total Environmental Burden through a scientific-based environmental-impact price.

(iii) An Extended Waste Management Pinch Analysis (E-WAMPA) system for regional planning, accounting for both burdening and unburdening footprints, to determine the waste treatments and allocation design with low emission footprints.

(iv) An assessment model underpinned by the P-graph tool to identify optimal and near-optimal integrated waste treatment systems for different waste compositions, which includes the identification of sustainable pre-and post-treatment processes.

The proposed methodologies, which can be represented graphically, with the support of a set of comprehensive underlying equations, transform the waste management and transport selection problem into an easily understandable format from which arises robust solutions with low emission footprints. As an example in one of the case studies, the analysis run by the novel approach using E-WAMPA suggests an overall 10 % emission reduction (2,568 kt CO2eq) can be achieved by performing waste transition in Malta (-25.75 kt CO2eq), Greece (-1,602.71 kt CO_2eq), Cyprus (-178.52 kt CO_2eq) and Romania (-761.16 kt CO_2eq). Those are the countries where the most improvement can be achieved, considering the combined effect of net emission (both burdening and unburdening footprints) by the existing waste treatment system, waste generation and population. For future study, a comprehensive economic feasibility assessment could be conducted, where localised data inputs could be fed into the proposed frameworks for a customised and thorough solution.

Abstrakt

Tato práce prezentuje metodologii snižování emisních stop v souvislosti s přechodem na oběhovou ekonomiku aplikováním integrace procesů při analýze a projektování při zohlednění výzev, které ztěžují praktické aplikace. Udržitelnost životního prostředí se vyznačuje snahou o snižování emisí a zlepšení hospodaření s odpady a hraje rozhodující roli při přechodu na oběhovou ekonomiku. Byly navrženy tři metodiky založené na bezztrátovém konceptu a rozšiřujících metodiky Pinch Analysis a P-Grafů. Aplikovatelnost je demonstrována šesti případovými studiemi transportu a nakládání s odpady. Mé příspěvky v této oblasti jsou následující:

(i) Nový bezztrátový rozhodovací nástroj paralelní s klasickým fázovým diagramem, který napomáhá rychlému rozhodování o procesech (např. výběr druhu dopravy pro danou vzdálenost a náklad) při nejnižší možné environmentální zátěži.

(ii) Systém kvantitativního vyhodnocování emisí, který agreguje a vyhodnocuje celkové environmentální zatížení způsobené sklemíkovými plyny, SO_x, PM a NO_2.

(iii) Rozšířená analýza nakládání s odpady pro regionální plánování s přihlédnutím k zatěžování i odstranění zatěžování emisní stopou, dále rozhodování o způsobu hospodaření s odpady a výběru způsobu zpracování odpadu s cílem nejnižší možné emisní stopy.

(iv) Model posuzování pomocí nástroje P-grafu pro identifikaci optimálních integrovaných systémů zpracování odpadu různého složení, který identifikuje a vyhodnocuje stav udržitelnosti procesů před a po zpracování.

Navrhované metodiky v grafickém znázornění s podporou sady komplexních základních rovnic transformují problematiku nakládání s odpady a výběru dopravy do snadno srozumitelné formy řešení vyznačujících se nízkými emisními stopami. Jako příklad v jedné z případových studií analýza provedená podle nového přístupu využívajícího E-WAMPA naznačuje, že celkového snížení emisí o 10% (2, 568 kt CO_2 ekv.) Lze dosáhnout provedením přechodu odpadu na Maltě (-25.75 kt CO_2 ekv.), Řecko (-1,602.71 kt CO_2ekv), Kypr (-178.52 kt CO_2ekv) a Rumunsko (-761.16 kt CO_2ekv). To jsou země, v nichž lze dosáhnout co největšího zlepšení, vzhledem k kombinovanému účinku čistých emisí (zatěžujících i nezatížených stop) stávajícího systému nakládání s odpady, vzniku odpadů a obyvatelstva. Následující studie budou umožňovat komplexní vyhodnocení ekonomické proveditelnosti tak, aby lokální data mohla být použita pro konkrétní případy v již předpřipravených schématech s výstupem kvalifikovaného řešení.

Acknowledgement

In completion of this thesis, it is most appropriate to reflect and recognise those individuals who have got me to where I am and express my gratitude. This thesis would not have been possible without the great support and guidance of my supervisor, Prof Jiří Jaromír Klemeš. His dedication and commitment in academics and research made him an excellent role model for the students. More than timely guiding with the theoretical aspects of my research, he promotes me and my work, provides opportunities, shares his experience and has fostered enormous growth in me. He has always been encouraging and believing in me before I believed in myself. I would also like to thank my co-supervisors, Prof Lee Chew Tin and Assoc Prof Simon Perry. I have learned a lot from Prof Lee, including soft skills and life lesson. Perhaps without her, I might not have the chance to meet Prof Klemeš. She has always been reachable and concern about my future development. I am grateful for the patience and time of Assoc Prof Simon Perry in contributing to the development and for editing my work.

I would also like to give sincere thanks to the co-authors of my several research papers, especially Dr Timothy Walmsley as well as Dr Petar Sabev Varbanov. There have been many inspiring discussions and technical suggestions which stimulated me to think from a different perspective. It has contributed significantly to the development of my research. I would also gratefully appreciate and recognise the financial support granted through the EU supported project Sustainable Process Integration Laboratory – SPIL funded as project No. CZ.02.1.01/0.0/0.0/15_003/0000456, by Czech Republic Operational Programme Research and Development, Education as well as the doctoral scholarship and extraordinary scholarship by VUT. There are others not associated directly with this thesis, but who have contributed, nonetheless. Here I wish to thank my colleagues and the Walmsley's family for their empathy, encouragement and most importantly all the together time in Brno as well as the helping hand of Dr Šárka Zemanová and Prof Stehlík with all the communication, supporting administrative work and help with the translation. A big shout out to my friends back in Malaysia and the other countries who were sparing their time to listen my stories and meeting me in Brno/Europe.

My biggest gratitude goes to my beloved family for their kind understanding, forbearance and endless support. The start of my PhD journey and the completion of this thesis would not be possible without their backing. Thank you for my parents for always letting me make my own decision and never interrupt me from doing what I wish. From them, you can see the spirit of you don't have to agree to support. Despite all the teasing, siblings are a blessing. I would like to thank sisters for their presence and always by my side.

Contributing Research Work Presented in Peer-Reviewed Publications

This thesis has been based on the author's publication in several highly recognised international journals. The developed methodology and work in Chapter 3 are published in Renewable and Sustainable Energy Reviews (IF: 10.566) [1] and Chemical Engineering Transactions [17]. Two publications closely related to the work in Chapter 4 are published in Chemical Engineering Transactions [16,18]. The results in Chapter 5 is based on the works accepted in Science of Total Environment (IF: 5.589) [2] and published in Journal of Environmental Management (IF: 4.865) [3]. The other review studies and assessments (waste treatment assessment, emission assessment, circular economy-related studies) that make up the thesis or developed the main results in Chapter 3 – 5 (result chapters) are published in Frontiers of Chemical Science and Engineering (IF: 2.643), Clean Technologies and Environmental Policy (IF: 2.277), Journal of Cleaner Production (IF: 6.396), Energy Conversion and Management (IF: 6.377), Journal of Environmental Management (IF: 4.865), Chemical Engineering Transactions (Scopus Index), and conference proceedings of various international conferences such as IEEE (Scopus Index). The complete list of publication is presented in this chapter as follows.

I have presented the research underpinning this thesis at 17 international conferences in Kentucky (USA), Stavanger (Norway), Adelaide (Australia), Delft (Netherland), Brač Island (Croatia), Bologna (Italy), Singapore, Tomsk (Russia Federation), Johor (Malaysia), Palermo (Italy), Prague (Czech Republic), Gangwon (South Korea), Krakow (Poland), Bangkok (Thailand), Dubrovnik (Croatia), Tianjin (China), Milan (Italy). The work in Chapter 4 was awarded best young scientist presenter (Session 1) in Sustainable and Efficient Use of Energy, Water and Natural Resources (SEWAN) conference, Tomsk, Russia Federation, 14 - 16 November 2018. I am also a co-author of several plenary and invited lectures, where the works have been presented by my supervisor at 20 international conferences in China, Croatia, Czech Republic, Hungary, Italy, Malaysia, Morocco, Poland, Russia Federation, Serbia, South Korea, Slovakia, Slovenia, Sweden, Taiwan, Thailand, Turkey and the United Kingdom. A complete list of the conferences and presentation is provided in the appendix (Table S2).

Journal Articles - Publication with Impact Factors

1. **Fan Y.V.,** Klemeš,JJ., Walmsley T.G., Perry, S. 2019. Minimising the Energy Consumption and Environmental Burden of Freight Transport using a Novel Graphical Decision-Making Tool. Renewable and Sustainable Energy Reviews, 114, 109335 **[IF: 10.566]**

2. **Fan Y.V.,** Klemeš, J.J., Walmsley T.G., Bertok, B., 2019. Implementing circular economy in municipal solid waste treatment system using p-graph, Science of Total Environment **[IF: 5.589] (Accepted)**
3. **Fan Y.V.,** Perry S.J., Klemeš J.J., Lee C.T., 2019, Anaerobic Digestion of Lignocellulosic Waste: Environmental Impact and Economic Assessment, Journal of Environmental Management.231, 352-363. **[IF: 4.865] (5 citations)**
4. **Fan Y.V.,** Lee C.T., Lim J.S., Klemeš, J.J., Le P.T.K., 2019. Cross-disciplinary Approaches Towards Smart, Resilient and Sustainable Circular Economy. Journal of Cleaner Production, 232, 1482-1491. **[IF: 6.396]**
5. **Fan Y.V.,** Perry S.J., Klemeš J.J., Lee C.T., 2018, A review on air emissions assessment: Transportation. Journal of Cleaner Production, 194, 673-684. **[IF: 6.377] (33 citations)**
6. **Fan Y.V.,** Klemeš J.J., Lee C.T., Perry S., 2018. Anaerobic digestion of municipal solid waste: Energy and carbon emission footprint. Journal of Environmental Management, 223, 888-897. **[IF: 4.865] (10 citations)**
7. **Fan Y.V.,** Klemeš J.J., Lee C.T., Ho C.S., 2017. Efficieny of microbial inoculation for a cleaner composting technology. Clean Technologies and Environmental Policy. 20(3), 517-527. **[IF: 2.277] (5 citations)**
8. **Fan Y.V.,** Varbanov P.S., Klemeš J.J., Nemet A., 2017. Process efficiency optimisation and integration for cleaner production. Journal of Cleaner Production. 174, 177-183. **[IF: 6.396] (16 citations)**
9. **Fan Y.V.,** Lee C.T., Klemeš J.J., Leow C.W., 2017. Evaluation of Effective Microorganisms on Small Scale Food Waste Composting, Journal of Environmental Management. 216, 41-48. **[IF: 4.865] (21 citations)**
10. Varbanov P.S., Walmsley T.G., **Fan Y.V.,** Klemeš J.J., Perry S.J. 2018, Spatial targeting evaluation of energy and environmental performance of waste-to-energy processing. Frontiers of Chemical Science and Engineering, 12 (4), 731-744. **[IF: 2.643]**
11. Hyman B., Ozalp N., Varbanov P.S., **Fan, Y.V**., 2019. Modeling energy flows in industry: General methodology to develop process step models. Energy Conversion and Management, 181, 528-543. **[IF: 6.377] (2 citations)**
12. Mardani A., **Fan Y.V.,** Shahbaz M., Nilashi M., Streimikiene D., Loganathan N., 2018. A soft computing approach for CO_2 emissions predicting based on renewable energy consumption and economic growth. Journal of Cleaner Production. 231, 446-461. **[IF: 6.396] (1 citation)**
13. Lee C.T., Haslenda H, Ho CS, **Fan Y.V.**, Klemeš JJ, 2017. Sustaining the low-carbon emission development in Asia and beyond: Sustainable energy, water, transportation and low-carbon emission technology. Journal of Cleaner Production. 146, 1-13. **[IF: 6.396]**
14. Lee C.T., Lim JS, **Fan Y.V.**, Liu X, Fujiwara T, Klemeš JJ, 2018. Enabling low carbon for sustainable development in Asia and beyond. Journal of Cleaner Production., 176, 726-735. **[IF: 6.396] (19 citations)**
15. Lee C.T., Rozali NEM, **Fan Y.V.,** Klemeš JJ, Towprayoon S., 2018. Low-carbon emission development in Asia: energy sector, waste management and environmental management system. Clean Technologies and Environmental Policy. 20 (3), 443-339. **[IF: 2.277] (6 citations)**

Journal Articles - Publication with Index

16. **Fan Y.V.,** Klemeš, J.J., Chin, H.H., 2019 Extended waste management pinch analysis (E-WAMPA) minimising emission of waste management: EU-28. Chemical Engineering Transactions, 74, 283-288.
17. **Fan Y.V.,** Klemeš J.J., Tan R.R., Vabarnov P.S., 2019. Graphical Breakeven based Decision-Making (BBDM) Tool to Minimise GHG Footprint of Biomass Utilisation: Biochar by Pyrolysis. Chemical Engineering Transactions. **(Accepted)**
18. **Fan, Y.V.,** Klemeš, J.J., 2019. Biomass supply and inventory management for energy conversion. Chemical Engineering Transactions. **(Accepted)**
19. **Fan Y.V.,** Klemeš J.J, 2019. Emission Pinch Analysis for Regional Transportation Planning Stagewise Approach. IEEE, DOI: 10.23919/SpliTech.2019.8783112
20. Klemeš J.J, **Fan Y.V.,** 2019. Internet of Things for green cities transformation: Benefits and challenges. IEEE, DOI: 10.23919/SpliTech.2019.8783076
21. **Fan Y.V.,** Klemeš J.J., Lee C.T., 2018, Pre-and Post-Treatment Assessment for the Anaerobic Digestion of Lignocellulosic Waste: P-graph, Chemical Engineering Transactions, 63, 1-6. **(4 citations)**
22. **Fan Y.V.,** Klemes J.J., Perry S., Lee C.T., 2018. An Emissions Analysis for Environmentally Sustainable Freight Transportation Modes: Distance and Capacity. Chemical Engineering Transactions, 70, 505-510. **(1 citations)**
23. **Fan Y.V.,** Perry S.J., Klemeš J.J., Lee C.T., 2018, GHG Emissions of Incineration and Anaerobic Digestion: Electricity Production Mix. Chemical Engineering Transactions, 72, 145-150. **(3 citations)**
24. **Fan Y.V.,** Lee C.T., Roswanira A.W., Lee S.C., Mohamad RS, 2017. Evaluation of Microbial Inoculation Technology for Composting. Chemical Engineering Transactions. Vol 56, 433-438. **(2 citations)**
25. **Fan Y.V.,** Klemeš J.J., Lee C.T., 2017. The update of anaerobic digestion and the environment impact assessments research. Chemical Engineering Transactions. Vol 57, 7-12. **(6 citations)**
26. **Fan Y.V.,** Klemeš J.J., Lee C.T., 2017. Challenges for energy efficiency improvement anaerobic digestion. Chemical Engineering Transactions. 61, 205-210. **(1 citation)**
27. **Fan Y.V.,** Lee C.T., Klemeš J.J., 2018. The Roles of Air Pollutants in Freight Mode Selection: Water Transportation. In 2018 OCEANS-MTS/IEEE Kobe Techno-Oceans (OTO) (pp. 1-6). IEEE.
28. Klemeš JJ, Vabanov PS, **Fan Y.V.**, Lam HL, 2017. Twenty years of PRES: Past, Present and Future-Process integration towards sustainability. Chemical Engineering Transactions, 61, 1-24. **(9 citations)**
29. Leow C.W., **Fan Y.V.,** Chua L.S., Muhamad I.I., Klemeš J.J., Lee C.T., 2017. A Review on Application of Microorganisms for Organic Waste Management, Chemical Engineering Transactions, 63, 85-90.
30. Bong C.P.C., Lim L.Y., Lee C.T., **Fan Y.V.,** Klemes J.J., 2018. The Role of Smart Waste Management in Smart Agriculture. Chemical Engineering Transactions,70, 937-942. **(4 citations)**
31. Klemeš JJ, **Fan Y.V.,** Varbanov PS, 2017. Sustainability and complex system thinking-process integration extensions. International Conference on Energy, Ecology and Environment. Stockholm, Sweden, 26-29 July 2017. [Proceedings]

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CHAPTER 1

INTRODUCTION

1.1 General Introduction

The Circular Economy (CE) has frequently served as a framework for system designs in recent various municipality and government strategy plans, especially in the European Union (EU). The CE stresses the need to close the material loop so as to achieve a no leakage design where waste management and transport planning play critical roles. This transition to a CE can be achieved by first minimising, and eventually eliminating, the material flow to the end of its life cycle by regenerating the material through reusing, recycling and recovering. The current measuring of the Circular Economy is based on a material flow accounting system (e.g. European Union material flow indicator, Japanese material flow indicator system, in-and output flows, circularity rate) for monitoring. However, environmental concerns about maintaining the circularity (ecological and emission impacts) deserve more attention. Korhonen et al. (2018) highlighted that scientific research is needed to quantify the actual environmental impacts of circular economy work towards sustainability as some of the circularity approaches can be energy-intensive. The wide debate on the environmental implication, benefits and trade-off of a more circular economy has also discussed by Mayer (2019). Quality of circularity (environmental footprint of the material flows) has to be considered rather than the over-emphasis on the degree of circularity of material flow. However, robust engineering design and a comprehensive assessment framework in facilitating the planning to achieve a sustainable circular economy transition is still lacking.

Environmental footprints have been the common indicators that are applied to quantify and assess environmental performance in recent years. Footprint indicators include carbon emission (GHG) footprint, emission footprint, water footprint, nitrogen footprint, land footprint, energy footprint and ecological footprint (Čuček et al., 2012). Among them, the GHG footprint has received significant research attention due to population growth and economic development related to the issue of climate change. Consequently, it has been subjected to global agreements, trade, and taxation. Figure 1.1 shows the GHG emitted by sectors in the EU. GHG emissions have been generally decreased except for transport which has increased by 223 Mt (26 %). The declining trend of GHG emissions in waste management (Figure 1.1) is mainly related to the decline in the methane contributed by the effort of avoiding waste going to landfill. More than 20 % of the total GHG emission is contributed by the transportation sector, and road transport has the highest share, see Figure 1.2. Transport (Dark blue) is also identified as the main contributor of most of the anthropogenic emissions such as CO, Pb and NO_x emissions as shown in Figure 1.3. It plays an important role in mitigating air emissions.

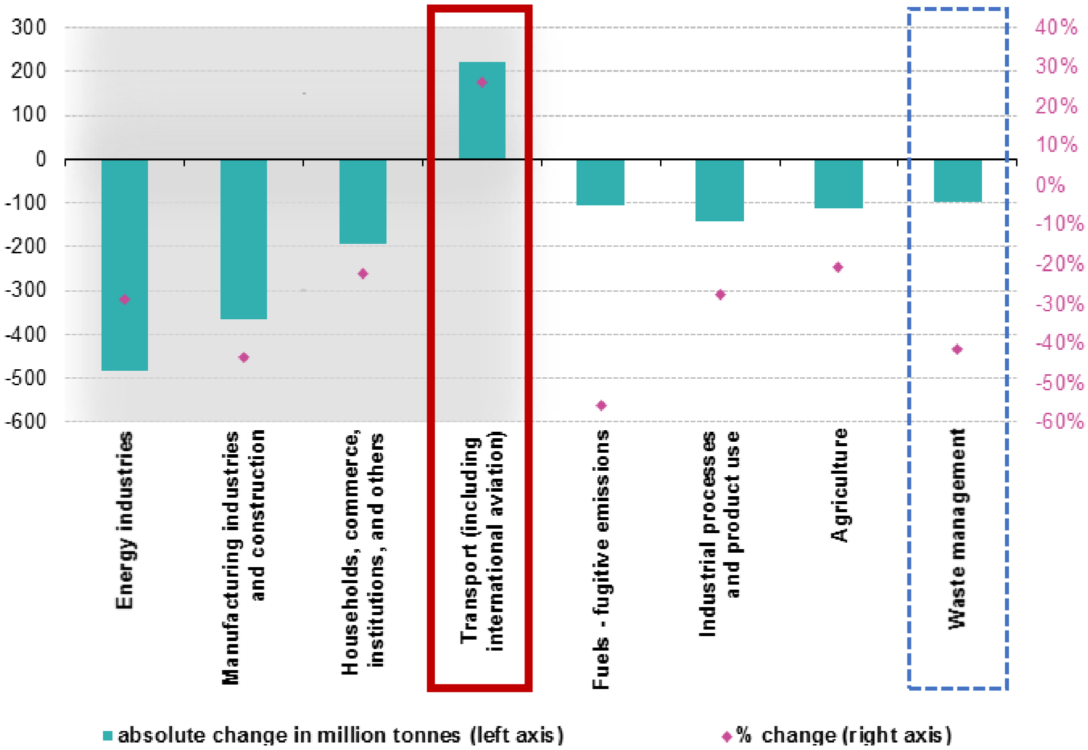


Figure 1.1: GHG emissions by IPCC source sector, EU-28 (Eurostat, 2018). Fuel combustion as a source of GHG emissions is indicated by the grey background shading

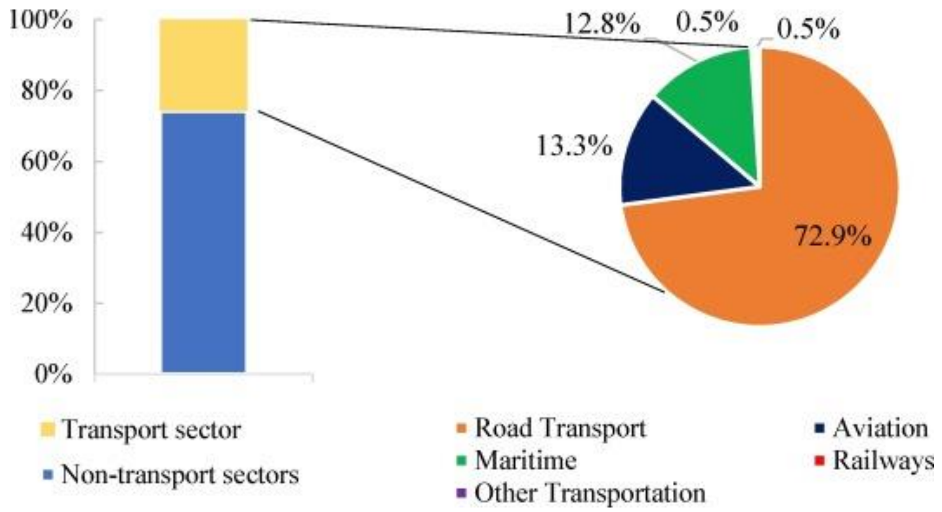


Figure 1.2: The GHG emissions by sources from the transport and non-transport sector in EU (Fan et al., 2018a)

The degree of circularity (both the material and ecological loops) can still be greatly improved (Haas et al., 2015) by enhancing the waste prevention and recovery effort, especially in the EU. This is reflected in the Circular Economy Package by the European Commission where various measures on waste have been proposed (EC, 2019) as well as in the inconsistent waste recovery performance across the EU members (Fan et al., 2019a). A common EU target, e.g. recycling 65 % of municipal waste, recycling 75 % packaging waste and reducing landfill to maximum of 10 % by 2030, as well as stimulating Industrial Symbiosis, has been introduced to enhance the progress of circular economy (EC, 2015). In this thesis, the selected case studies to demonstrate the developed methodologies for low emissions planning are focused on waste treatment/ management and transportation activities with the consideration of its roles in CE and as one of the largest emitters (GHG and non-GHG).

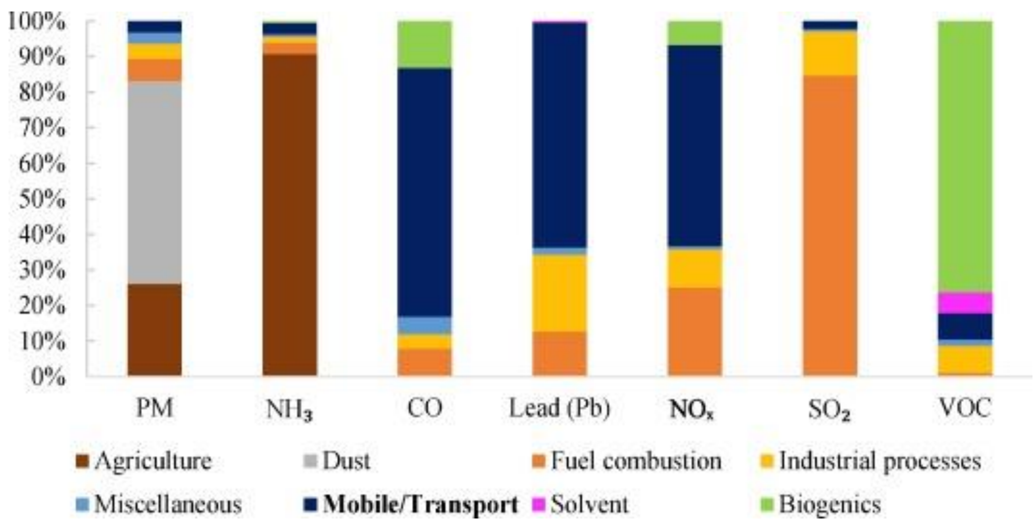


Figure 1.3: The pollutant emission comparison by source sector in the US (Fan et al., 2018a)

However, in comparison, air pollutants have received far less attention in defining the environmental sustainability of processes and systems. It is commonly noticed that environmental sustainability has been simply represented by CO_2 emission/GHG/Carbon footprint in most of the optimisation assessment and performance analysis (Fan et al., 2018a). Initiatives that protect the environment (air emissions) should be focused on an overall system rather than the choice of either clean air or mitigating climate change. Reduction of air pollutants is proposed as the co-benefits of the GHG mitigation (Zhang et al., 2016) with the explanation that the sources of emissions are the same. However, this relationship does not apply in all circumstances. The importance of incorporating air pollution measurement while developing climate change control policies was highlighted by Slovic et al. (2016). This is especially the case in the transportation sector, which is at the heart of the supply chain. A network or process design with low GHG emissions may not be an optimised solution when air pollutants (e.g. NO_x, SO_x, Particulate Matter - PM) are considered. A methodology to measure GHG and air pollutants simultaneously by considering the synergistic effect is therefore needed. It is crucial for minimising the potential of footprint shifting and poor decision-making.

Process Integration (PI) is a method of taking a holistic approach to process design and optimisation that looks at how a collection of processes or system are best integrated (Linnhoff, 1994). It can be defined as a systematic and general method for designing an integrated production system ranging from individual processes to Total Sites and with particular emphasis on the efficient use of energy and reducing environmental effects (Klemeš, 2013). This concept can form a foundation from which to embed sustainability (emission reduction) and Circular Economy into system design. Pinch analysis (Linnhoff et al., 1982) is among the standard approach/technique of PI. This targeting approach with graphical representation is suitable for practical purpose, easier to understand by the practitioner and serve as an excellent platform in minimising the problem size for the subsequent detailed planning. Pinch analysis remained highly relevant, even though mathematical programming techniques can also be used to resolve similar problems (Tan and Foo, 2007).

Another possible tool for low emission process design in a circular economy is the P-Graph. The approach of the P-graph technology differs considerably from conventional generic optimisation methods. It has proven useful in solving problems in supply chain management, discrete event decision making, reaction pathways identification, and energy conversion, as highlighted by Varbanov et al. (2017). The advantages of choosing the P-graph over other mathematical programming tools are the use of a graphical user interface for inputting maximal structures and displaying results, the emphasis on structural optimisation leading to optimal and near-optimal solutions and the software is open-source (Walmsley et al., 2018). The consideration of the near-optimal solutions is an important feature for low emission planning as it is difficult to capture in a mathematical model a high-fidelity representation of the real situation because of uncertainties, subjective parameters and weightings, and many practical constraints.

Research studies that have applied these tools/methods (e.g. Pinch Aanalysis, P-graph or graphical approaches) to minimise the emission footprints in waste management and transportation activities are still underdeveloped. Mathematical optimisation is the common approach, but the models developed still have a limited concern on non-GHG emission and integrated design. It is also comparatively difficult to understand the reason for obtaining the optimal solutions and communicate the results to decision-makers as specific mathematical modelling knowledge is needed. This study proposes three novel methodologies (i. Novel graphical tools based on a breakeven concept, ii. Extension of Pinch Analysis, iii. P-graph based model), considering integrated solutions and non-GHG emissions in identifying a low emission footprint design for waste management and transporting activities.

1.2 Thesis Aim and Scope

The overall aim of the research is to investigate and develop methods to minimise the emission footprints in the circular economy by Process Integration. Robust engineering design and comprehensive assessment framework in facilitating the planning to achieve emission reduction are proposed. The research in this thesis fills the following research gaps:

i. The circular economy concept currently still lacks robust engineering design methods and quantification. The net environmental footprints (e.g. emission) in maintaining the circularity needs to be assessed as additional utilities or resources are required.
ii. The available decision-making models primarily use the perspective of GHG footprint to represent environmental sustainability. It deserves more development to consider additional emission footprints.
iii. Most of the proposed decision models use a mathematical programming method where the studies based on a graphical approach for low emission footprints decision making and systematic planning are comparatively scarce.
iv. Embedding of Process Integration thinking (e.g. Integrated regional planning, Integrated treatments, Integrated emissions) in system design is still lacking.

Waste management and transportation activities are the targeted sectors, and case studies have been developed related to these sectors to demonstrate the developed methodologies. Three novel methodologies are proposed and applied to six case studies. The scope of the study is divided into the following main sections:

i. **A breakeven based decision-making tool for low emission planning**

To develop a novel graphical tool based on the breakeven concept in facilitating the selection of processes (transportation, pyrolysis - biomass utilisation) with the lowest emissions possible. GHG, NO_x, SO_2, and PM are aggregated by environmental price as a Total Environmental Burden (TEB). The breakeven border or points defines when two or more processes would have equivalent emissions. The area above or below the breakeven is assigned to different options representing the circumstance where the options have the lowest emissions. It provides a rigorous basis for decision support.

Case Study 1: Transportation

Identification of low emission transportation solutions (e.g. heavy lorry, light lorry, container ship, cargo ship, train) under different circumstances (e.g. load and travelled route/distance) for different scenarios (e.g. EU-28, Latvia, Sweden; transports powered by electricity, diesel, biodiesel, compressed natural gas and liquefied natural gas). The comparison of solutions with the lowest GHG emission and lowest TEB.

Case Study 2: Pyrolysis of Biomass

Identification of optimal biomass utilisation (to burn or to bury the biochar) where the lowest GHG emissions and the highest possible profit indicate the optimal choice. Different type of biomass (energy crop, agricultural residue), GHG pricing (carbon tax) and carbon emissions intensity of a country are assessed.

ii. **Pinch Methodology to minimise the emissions of waste management system through integrated regional planning**

To extend the methodology of Waste Management Pinch Analysis for integrated regional planning where the resources/waste, as well as the facilities/infrastructures at different places, can complement each other to achieve a lower net emission (consider both burdening and unburdening life cycle emission) design.

Case Study 1: Integrated Regional Municipal Solid Waste Management

Determination of the waste management system (a set of waste treatments) for EU countries to achieve a defined emission reduction target. The emission reduction strategy is treatment transition. The priorities of this transition are targeted on the EU countries with high net GHG emission (contributed by waste management) per capita. The net emission per capita considering the waste amount, population and waste treatment practices (both burdening and unburdening footprints) for comparison. Introduce waste trading to further reduce the emission footprints, with the concept that the waste (after optimised in their own region/country level) at a place can be a resource of other places.

Case Study 2: Integrated Regional Biomass Inventory and Sourcing Management

Identification of optimal production rate, inventory, storage and biomass network flow (sourcing) with the lowest possible cost incurred in transporting and carbon tax (environmental price). The developed Pinch methodology for targeting is integrated with a mathematical model for subsequent optimisation. The seasonal availability of supply and demand for biomass (surplus and deficit at different time frame) is overcome through integration planning.

iii. P-graph structure to assess the waste treatment design with minimal emission.

To develop a maximal structure by using the P-graph in identifying an integrated design (integrated waste treatment system, pre-and post-treatment) with minimal emission footprints and maximum profit. The optimisation approach can capture both optimal and near-optimal solutions. It offers more rational synthesis decisions.

<u>Case Study 1: Waste Treatment System</u>

Identification of suitable treatment system for municipal solid waste (MSW) by considering the economic balance between the main operating cost, type, yield, quality of products as well as GHG emission. Four types of MSW composition by country income level are investigated. The impacts of altering the price of biofuel, digestate, compost, GHG, electricity and heat to the suggested integrated treatments are evaluated.

<u>Case Study 2: Pre-and Post-Treatment</u>

Identification of optimal pre-and post-treatment for anaerobic digestion by considering the cost and environmental performance. The assessed substrate is a lignocellulosic waste, where up to 16 treatments have been assessed. Global warming potential, human toxicity, ozone depletion potential, particulate matter, photochemical oxidant creation, acidification and eutrophication potential are measured in defining the environmental performance.

1.3 Thesis Outline

Chapter 2 thoroughly reviews the key literature and advances of the available methodologies that are most relevant to the aim of this thesis. The main research comprising this thesis is divided into three chapters (Chapter 3 - 5), where three novel methodologies are developed and presented. The applicability of the proposed methodologies is demonstrated through 6 case studies related to waste management and transportation. Each of the case studies provides specific results (see Chapter 3 - 5) of the assessed scope (see Section 1.2), which could significantly contribute to the field of study. Chapter 6 overviews the contribution of this thesis with a recommendation for future work, followed by references and appendix.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter presents the literature relevant to the thesis aim. Figure 2.1 summarises the keywords and sections of this chapter. Section 2.2 provides a brief introduction of the Circular Economy follows the research gaps for the transition of this system. The environmental footprints, specifically the emission footprint, in maintaining or creating the circular system, have to be considered. Section 2.3 discusses on emission footprints and the available environmental pricing/tax. Section 2.4 reviews the current decision making and low emission process design approaches as well as the limitation. The discussion is divided into two subsections focusing on waste management (Section 2.4.1), and transportation (Section 2.4.2) arises from their critical roles in narrowing the material loop. Section 2.5 and 2.6 introduce Process Integration (e.g. Pinch Analysis, and other graphical approach) and P-Graph framework. The research gaps and their potentials in achieving the thesis aim are highlighted.

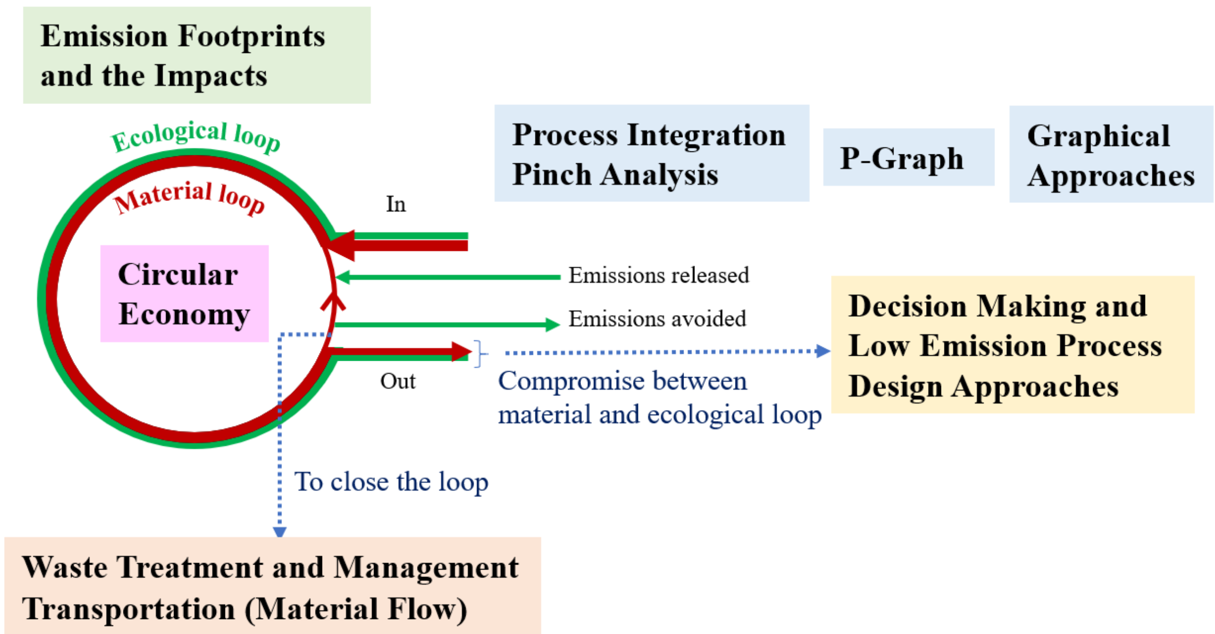


Figure 2.1: The outline and keywords comprise of the literature review

2.2 Circular Economy

Circular economy was introduced as an economic or business model for the transition of linear to a circular system. One of the main issues of closing the circular economy loop is transforming waste into secondary raw materials. It has risen in popularity in recent years as a conceptual model to guide better use of natural resources and management of waste (Murray et al., 2017). The utilisation of waste as resources can scale down the demand for extraction of new resources and avert the impacts created along the processing chain. This is critical to support the transition from a linear to a circular economy. The circular system can be achieved by avoiding the material flow to the end of the life cycle (reducing) or by regenerating the material through reusing, recycling and recovering.

There have been various definitions for the circular economy as summarised by Suárez-Eiroa et al. (2019). Kirchherr et al. (2017) highlighted the variety of understanding in the circular economy concept, and a lack of quantification approach can end up in a conceptual deadlock. According to one definition, a circular economy is a system developed by minimising the use of energy, natural resources and waste generation (Tura et al., 2019). It can be achieved by mitigating, closing and narrowing loops of utilities and materials flows. Based on a conducted systematic analysis, most scholarly see the circular economy as an avenue for economic prosperity (Kirchher et al., 2017) and a material or energy flow balance. Rather than having circularity as a goal, a more pragmatic vision for a material future would be aimed to meet human needs (demand) while minimising the environmental impact. This is in line with the conclusion by Korhonen et al. (2018), highlighting scientific research is needed to secure the actual environmental impacts of circular economy work towards sustainability as some of the circularity approaches can be energy-intensive. The environmental concern of maintaining the circularity has been gradually embedded to the traditional concept in the recent year but still deserves more attention. One of such approaches is the Circular Integration Framework proposed by Walmsley et al. (2019). However, the considered environmental performance demonstrated in the study is only the GHG footprints where usually consistent (e.g. low energy consumption equivalent to low GHG footprint) with the energy input-output balance.

There have been various single and composite indicators to define environmental performance. Environment impacts include the mid-point, and end-point categories are well established in life cycle assessment (LCA). These include global warming potential, acidification, eutrophication, photochemical ozone creation potential, toxicity and human health etc. (Jolliet et al., 2003). Environmental footprints are the common indicators that applied to quantify and assess environmental performance in recent years. The footprints indicators include carbon emission footprints, water footprint, nitrogen footprint, land footprint, emission footprint, energy footprint and ecological footprint (Čuček et al., 2012). Carbon emission footprint and global warming potential are among the most considered impact and received great concern due to the climate change issue that subjected to global agreements, Intended Nationally Determined Contributions as summarised in Lee at al. (2018), and taxation.

The current indicators of the circular economy, on the other hand, are more specify on material flow accounting system which usually derived based on European Union material flow and Japanese material flow indicator system (Geng et al., 2012). The sustainability is not within the concern of such accounting. The other material flow accounting derived indicators based on regional nuances and policy are a) energy and material efficiency indicator in Korea and b) decoupling of material flow intensity in the United States. In China, the circular economy evaluation system covers a more extensive range of consideration include resources output and consumption rate, integrated resource utilisation rate, waste disposal and pollutant emission. Haupt et al. (2017) apply recycling rates as an indicator to measure the degree of circularity of the Swiss waste management system. Nakamura and Kondo (2018) developed a dynamic waste input-output model. Circular material use rate is proposed by Eurostat (2018) to measure the share of material recovered and fed back into the economy. The promotion of circularity without considering the environmental footprints in the accounting could lead to the crisis or adverse effect as the plastic recycling issues. Waste is exported to a developing country for creating/pushing a high recycling rate. A similar issue has been highlighted by Pauliuk (2018) in reviewing the circular economy standard BS 8001:2017, stating the need for the established accounting and assessment tools for material flows, environmental and social impacts.

A set of indicators comprise of a) scale indicators (t) (In-and output flows, consumption-based perspective, interim flows), and b) circularity rate (%) (socioeconomic cycling, ecological cycling potential, non-circularity) has been proposed by Mayer et al. (2019) to identify the circularity of EU. As shown in Figure 2.2, only 0.71 Gt of the processed materials are from secondary materials, contributed to a low output socioeconomic cycling rate (OSCr) of 14.8 % (Figure 2.3). The input socioeconomic cycling rate (ISCr) is even lower (9.6 %) suggested that not all the reprocessed secondary material is utilised in the domestic economy. This study highlights the roles of waste recovery in a circular economy and the need for systematic waste management planning.

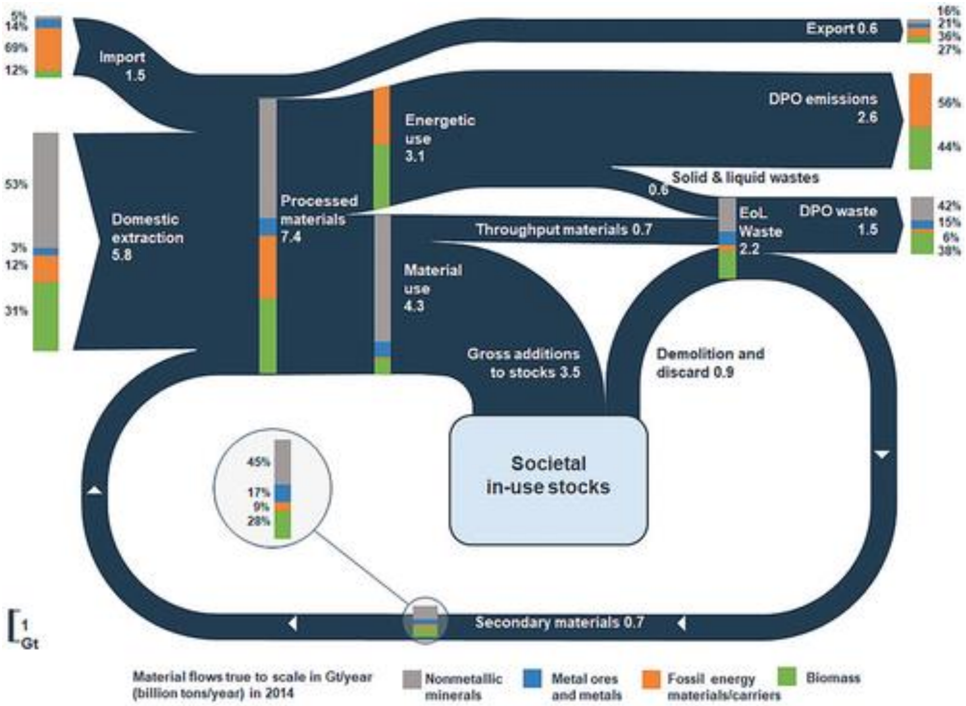


Figure 2.2: Material flows through the EU28 economy. Mayer et al. (2019). (Domestic processed outputs = DPO. EoL = End of life)

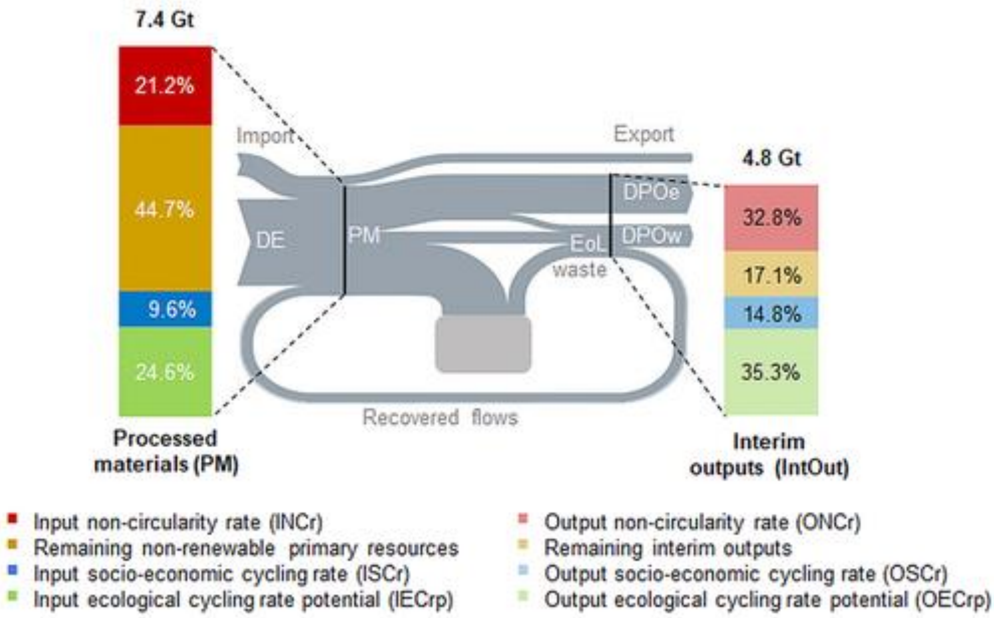


Figure 2.3: Input and output side circular economy indicators of EU28 (Mayer et al. (2019). Socio-economic cycling rate shows the share of secondary material in processed materials. Ecological cycling rate shows the share of domestic material consumption of primary biomass in the processed material. Non-circularity rate shows the share of energetic use of fossil energy carriers in the processed material. DE = Domestic extraction, PM = Processed material. DPOe = Domestic processed output of emission. DPOw = Domestic processed output waste.

The proposed indicators are relatively comprehensive; however, they only serve as a monitoring framework (system assessment tools instead of system engineering model) in this study. The results inform the circularity situation of EU. The consideration of environmental footprints is still limited and is not initially designed to facilitate the material/ waste management planning. It does not provide insight into how the waste management system of among the EU members can complement each other in achieving a quality circular economy (meet the emission reduction target, etc.).

To summarise,

i. The environmental footprint of the material flows (quality of circularity) has to be considered rather than over-emphasising on circularity (degree of circularity).
ii. Material flow and waste management are the keys of the circular economy
iii. The circular economy concept still lacks robust engineering design and comprehensive assessment framework in facilitating the planning to achieve a defined target (e.g. circularity rate, emission/ footprints reduction target)

2.3 Emission footprints and Environmental Prices

Emission footprint can be generally defined as the quantities of product or service-created emissions into the air, water and soil (Čuček et al., 2015). The conversion of emissions is calculated based on the principle that anthropogenic mass flows must not alter the quality of local compartments where maximum flows are defined based on their replenishment rate per unit area (Bendedetto and Klemeš, 2015). In most of the cases, the focus of emission footprint is given to the air emissions due to the global concern as well as the existence of other footprints in quantifying the emission to the water and soil, e.g. water footprint, land footprint, ecological footprints. The emission footprint discussed in this study is focused on air emissions where the GHG (climate change) and air pollutants (e.g. SO_2, NO_x and particulate matter) are both considered. GHG and CO_2eq is the common term and unit used for describing the gaseous contribution to climate change. In contrast, it is comparatively complex to have a common term or unit for air pollutants. A composite term or unit, despite having some deficiencies (USAID, 2014) on the accuracy of representation (in assigning the weighting factor), it facilitates the optimisation assessment and simultaneous assessment (air pollutants with GHG) by having multiple attributes in a composite form as well as being easy for communication. Studies that have measured air emissions from transportation have been based on a wide variety of methods. The methods of identifying the air emissions were divided into primary (direct measurement, direct measurement at source point) and secondary (emission factor, modelling) as summarised in Table 2.1.

Table 2.1.: Comparison between the approaches to obtain the input data for LCA and optimisation study

Parameters	Input Data for Emission Assessment- The Measurement Method			
	Primary (Experimental)		Secondary	
	[1]Direct measurement (DM)	[2]Direct measurement at the source point	Emission factor (EF)	Modelling
Uncertainty	Lower	Lower	[3]High	[3]High
Time taken (Analyse/ Calculate)	Longer	Shorter than DM	Short	Short
Cost	Higher	High	Lower	Lower
	The Other Characteristics			
Merits	Measure the secondary emissions/ pollutants Could be real-time display	Consider the real-world performance. Real-time display	Simplicity	Predict alternative situations/ scenario by include different factors e.g. wind (Meteorological)/ Secondary pollutants
Demerits	All the emission in the air, e.g. including sea spray, is included, source detection step is needed. [5]Do does not represent a real-world situation.	[4]Calibration is needed. Could vary by device. Low reproducibility	A secondary pollutant is usually not included. [6]Sensitive/ localised, need to update from time to time	Rely on accurate input Localised

[1]Two different type of direct measurement, refer to the explanation in text. [2]Refer to the onboard measurement (e.g. device attached to the transport mode). [3]Depend on the scope and boundary in determining the EF, suitability/ compatibility (e.g. type of engine) and rely on accurate input (See grey line in Fig. 7). [4]EURAMET (2017). [5]The limitation of direct measurement conducted in an experimental controlled condition at the laboratories. [6]Refer to text for a detailed explanation.

Emission factor (EF) is one of the most common methods to obtain input data for assessment studies due to its simplicity and is summarised in Table 2.1. The uncertainty is high as the EF is usually cased specifically with some factors being excluded. Table 2.2, Table 2.3, shows the emissions factors (GHG and air pollutants) of different freight transportation modes.

Table 2.2.: The GHG emission factor of different freight transports (Road, sea, inland and rail)

Mode of Transportations	Emission factor (g/t-km) of GHG Round off to 4 decimal places (D.P)			
	CO_2eq[1]	CO_2	CH_4	N_2O
Road/Truck (Delcampe, 2014)		110		
Truck >32 t (EEA, 2014)		102	0.001	0.004
Truck-Lowest (OECD, 1997)		127		
Truck – Highest (OECD, 1997)		451		
Truck (Facanha and Horvath, 2007)		116.1967		
Truck-Trailer (Boer et al., 2017)	192			
Truck >20 t (Boer et al., 2017)	**337**			
Sea (Delcampe, 2014)		7		
Sea (OECD, 1997) Lowest		30		
Sea (OECD, 1997) Highest		40		
Sea (Boer et al., 2017)	**58**			
Inland (Delcampe, 2014)		49		
Inland (EEA, 2014)		53	0.007	0.002
Inland (Boer et al., 2017)	51			
Rail (Delcampe, 2014)		35		
Rail (EEA, 2014)		52	0.004	0.002
Rail (OECD, 1997) Lowest		127		
Rail (OECD, 1997) Highest		451		
Rail (Facanha and Horvath, 2007)		24.8549		
Rail-Electric, Medium-length (Boer et al., 2017)	39			
Rail-Diesel, Medium length (Boer et al., 2017)	73			

[1]CO_2eq, CO_2 equivalent emissions in this study refer to CO_2, CH_4 and N_2O. Unit Conversion: 1 mile=1.60934 km, rounded off to 4 decimal places.

Table 2.3.: The air pollutants emission factor of different freight transports (road, sea, inland and rail)

Mode of Transportation	Emission factor (g/t-km) of air pollutants (Round off to 4 D.P)							
	CO	NMVOC	VOC	HC	NO_X	PM_{10}	PM	SO_2
Road/Truck >32 t (EEA, 2014)	0.18	0.016	0.018		0.57	0.01		0
Truck-Lowest (OECD, 1997)	0.25		1.1	0.3	1.85		0.04	0.1
Truck - Highest (OECD, 1997)	0.4		1.1	1.57	5.65		0.9	0.43
Truck (EEA, 2011)	0.2		0.1		0.92		0.02	
Truck (Facanha and Horvath, 2007)	0.3728				1.5969	0.2175		0.0932
Truck-Trailer (Boer et al., 2017)					2.2	0.031		0.2
Truck >20 t (Boer et al., 2017)					**1.1**	**0.019**		**0.35**
Sea-Lowest (OECD, 1997)	0.018		0.04	0.04	0.26		0.02	0.02
Sea-Highest (OECD, 1997)	0.2		0.11	0.08	0.58		0.04	0.05
Sea (EEA, 2011)	0.03		0.01		0.33		0.03	
Sea (Boer et al., 2017)					**0.99**	**0.023**		**0.087**
Inland (EEA, 2014)	0.82	0.267	0.274		1.24	0.058		0.274
Inland (EEA, 2011)	0.03		0.03		0.6		0.04	
Inland (Boer et al., 2017)					0.065	0.025		0.054
Rail (EEA, 2014)	0.07	0.025	0.029		0.3	0.01		0.014
Rail-Lowest (OECD, 1997)	0.02		0.08	0.01	0.2		0.01	0.07
Rail-Highest (OECD, 1997)	0.15		0.08	0.07	1.01		0.08	0.18
Rail (EEA, 2011)	0.03		0.04		0.14		0.01	
Rail (Facanha & Horvath, 2007)	0.2610				0.4598	0.031		0.074
Rail-Electric, Medium length (Boer et al., 2017)					0.037	0.002		0.021
Rail-Diesel, Medium length (Boer et al., 2017)					0.787	0.024		0.075

The wide range of emission factors among the same mode is due to the diverse assessment boundary and approaches (e.g. tailpipe emission, combustion emissions, evaporative emissions, wear processes, other emissions like heavy metals and Polycyclic aromatic hydrocarbons from leakage of engine oil) (Klein and Fortuin, 2014), technology development, fuel (e.g. renewable energy) as well as engine efficiency. The real-world condition, e.g. on the road (gradient), ambient and driving conditions can vary over a wide range causing the EF to be higher than EF measured in the laboratory. Other factors that contribute to the high uncertainty of applying EF as input data include emissions deterioration over the useful life of the vehicles, emissions characteristics varying among identical engines, as well as the impact of cold and hot start (engine) (JRC, 2017).

The EF presented in Table 2.2, Table 2.3, does not provide a whole picture on which freight transportation mode provides lower emissions. Other than the high variation of reported data, more importantly, distance and load have a substantial effect on the emissions. Distance travelled by different transportation mode (e.g. road vs sea transportation) has a significant impact on decision making. The process design (or transport mode) with the lowest GHG emissions are not always a selection with the lowest air pollutants (non GHG) emissions. A methodology, preferably in graphical, to achieve fair comparison in assessing the impact of GHG and air pollutants of different transporting activities is needed. The reported EF of different transport modes and emission types is an average EF. It is important to consider the marginal emission contributed by the goods and the fix emission by the empty vehicle. This issue has been raised by Bigazzi (2019) in highlighting the probability of leading to a bias decision making. The models proposed in this thesis take marginal emission into the account (transportation-related accounting) as well as the burdening and unburdening emission. Burdening and unburdening emission (Kravanja and Čuček, 2013) are particularly for waste management case studies. The released (burdening) emission along the treatment processes and the avoided (unburdening) emission from the recovered product or utilities are both accounted for.

Simultaneous assessment of GHG and air pollutants (In this study, defined as emission footprints) is challenging due to their different impacts on the environment and having a different atmospheric lifetime. GHG is the main contributor to climate change, and air pollutants threaten human health. The further interaction of air pollutants in the atmosphere contribute to the formation of haze/smog as well as acid rain. Including air emission components with the other critical criteria in the decision making is rather complicated.

Multicriteria optimisation has been commonly applied to overcome the difficulty in evaluating the criteria with different impacts. The weighting factors assigned based on expert's judgement or survey experiences a certain level of uncertainty. This approach relies naturally on the weighting impact. The chosen weighting factors significantly influence the results or solutions.

Price is one of the means to integrate economic and environmental concern in an assessment. The advantage of this means is that it can directly be incorporated together with a given economic objective (or emission with different impacts) within the objective function. The subjective weighting between sustainability objectives can be avoided (Klemeš, 2015). Carbon pricing is one of the most common external cost with the aim to stimulates clean process design. The two main types of carbon pricing are an emission trading system (or cap-and-trade system) and carbon tax. The difference of this pricing system is that the emission reduction outcome of a carbon tax is not pre-defined, but it is for emissions trading system (market price). World Bank (2018) provides a comprehensive summary of the state and trends of carbon pricing in different countries. The carbon price ranges from 1 to 139 USD/ tCO_2eq., where the highest prices are by Sweden (139 USD/ tCO_2eq) follows by Switzerland (101 USD/ tCO_2eq) and Finland (77 USD/ tCO_2eq) (World Bank, 2018).

Eco-cost and environmental prices are another environmental dimension expressed as monetary values. Eco-costs are the cost of the environmental burden of a product on the basis of prevention of that burden (Vogtländer et al., 2002). Environmental prices are indices expressing the willingness to pay for less environmental pollution (CE Delft, 2018). The consideration is not limited to climate change or global warming potential. Table 2.4 summarises the pricing values of eco-cost and environmental price in the EU. Environmental prices as damage cost are generally higher than eco-cost. The midpoint impact (e.g. climate changes, acidification, human toxicity), as well as the damage caused at endpoints (human health, ecosystem services, wellbeing, resources availability, materials), are considered, as stated in CE Delft, (2017). The advantage of this single indicator simple and transparent calculation and easy for communication.

Table 2.4: Eco-cost and Environmental Price

Eco-cost[a,b]	Environmental Price
8.75 €/kg SO_x equivalent	11.5 €/kg (SO_2)
(acidification)	
6.0 €/kg NO_x equivalent	14.8 € / kg (NO_x)
(Summer smog)	
35.0 €/kg fine dust PM2.5 equivalent	26.6 €/kg (Particulates, < 10 um)
(Fine dust)	38.7 €/kg (Particulates, < 2.5 um)
0.116 €/kg CO2 equivalent	0.057 €/kg (CO_2)
(Global warming)	Methane 1.74 €/kg (CH_4)

References: [a]TU Delft, (2019); [b]Vogtländer et al. (2002); [c]CE Delft, 2018

To summarise, environmental pricing is one of the effective ways to aggregate GHG, air pollutants and cost (economic perspective) under one objective for optimisation. This approach enables better solutions and represent prices by adequately accounting for environmental (or in this thesis, air emission) problem. It is essential to identify the marginal emissions and consider the distance and load to be transported for better decision making (selection of transport type and mode). Unburdening emission should be taken into account in the emission accounting of waste management related activities.

2.4 Decision Making and Low Emission Process Design Approaches

There have been various system engineering and assessment model for decision making and process design. The discussion in this section is divided into two parts, focusing on the approaches for waste treatment and management (Section 2.4.1) as well as transportation (Section 2.4.2).

2.4.1 Waste Treatment and Management

Material/ waste management planning plays an important role in closing the economic loop as well as the environmental footprints (e.g. emissions) loop. Improper material/ waste management contributes to environmental issues such as greenhouse gas (GHG) emission, air, ground and water pollution. It is increasingly recognised that the growing metabolism of society is approaching limitation with respect to sources for resource inputs and sinks for waste and emission outflows (Haas et al., 2015). A wide range of waste recovery approaches includes material recycling, waste to energy (incineration, anaerobic digestion, gasification, pyrolysis, sanitary landfill) and biological recovery (composting) have been introduced to support continuing economic growth and industrial development. The initiatives to support the circularity system; however, consumes energy and contribute to environmental footprints in the process of mitigating the footprints of the waste ended in a landfill. This section assesses the available systematic planning methodologies to support the decision making of a waste management system from the environmental perspective. The focused issues are waste treatment selection.

The compositions and characteristics of waste vary for different cities, countries and regions. An adequate design of waste management system is highly dependent on the waste amount, the composition of the waste (Ghinea et al., 2016), current waste separation practices in place, resources, infrastructure and facilities. Various approaches have been applied to identify suitable waste treatment options and management systems. It can be generally divided into heuristic methods, multi-criteria decision analysis, graphs and network theory, mathematical optimisation, stochastic process techniques and statistical methods as summarised in the review by de Souza Melaré et al. (2017). Morrissey and Browne (2017) stated that the decision-making models that apply in waste management are divided into three categories (1) cost-benefit analysis, (2) LCA and (3) multi-objective approach.

A better classification has been presented by Cobo et al. (2018). Those authors classified the approaches in waste management studies into two major groups: system engineering models and system assessment tools. System engineering models focus on supporting the design of the system, while system assessment tools focus on evaluating the performance of the existing system. Sustainability analysis requires an integration of these two approaches. A detailed review of system analysis for solid waste treatment has been done by Chang et al. (2011), where the technology hub is presented (Figure 2.4). The five systems engineering models (in the circle, LP, DP, MIP and NLP are optimisation model) can be served as the core technologies where the model-based decision support system can be constructed for separate or collective applications. Chang et al. (2011) stated that the graphical decision support systems or expert systems can still be formed according to heuristic approaches using the rest of system assessment tools (the 8 triangles).

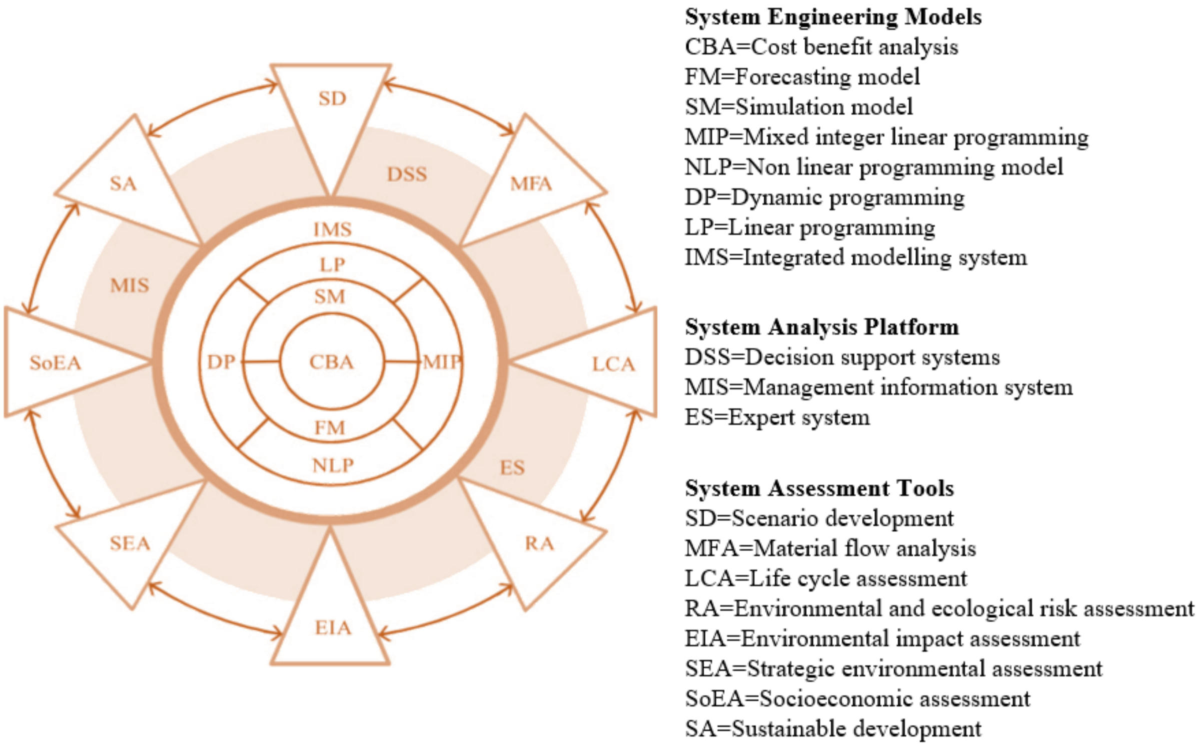


Figure 2.4: The technology hub for waste management system analysis. Adapted from Chang et al. (2011).

Many studies focus on scenario analyses for a sustainable waste management system. A different mix of waste treatment technologies, such as landfill, incineration, recycling, composting and other waste-to-energy (options) technologies, are modelled through scenario analyses. Estay-Ossandon et al. (2018) applied fuzzy TOPSIS-based scenario analysis to improve WSM planning and forecasting. The model also estimates the annual ratios to be reached for each waste processing so that they can comply with the European Directive. Some studies also considered a multiple-period planning to provide varied scenarios at different time frames, taking into consideration the demand and supply side of the waste inputs (e.g. increased waste volume of varying waste types), outputs (e.g. energy, compost, recyclables) and policy implication with time (Tan et al., 2014).

Assessment from an economic perspective has received the most research attention as it is the primary concern of treatment system implementation. With the growing concern on sustainability, environmental impacts have also received considerable attention. Life cycle assessment (LCA) is commonly applied to identify waste management and treatment systems with minimum environmental impacts. It identifies the environmental impacts of all process stages, including energy use and production; providing information from an integrated viewpoint. Dong et al. (2014) assessed the environmental impacts of three different treatment scenarios (landfill, landfill with landfill gas collection and incineration with energy recovery) in Hangzhou, China by using the LCA framework. Cremiato et al. (2018) assessed the environmental impacts of different waste separation and treatment approaches as an extension of previous techno-economic analysis (Zaccariello et al., 2015). The results of the LCA highlight the importance of waste separation and recycling. Milutinović et al. (2017) assessed several environmental impacts of four different waste management scenarios through the LCA and multi-criteria approach. Anaerobic digestion with biogas utilisation is suggested as the adequate option for Niš, a city in Serbia. A similar study has been done by Coventry et al. (2016) for Austin, Texas, USA. These studies focused on analysing the implementation of a single treatment approach with the possibility of an integrated multi-treatment system. An integrated waste management system is considered in the study by Parkes et al. (2015) for the London Olympic Park. However, the assessment is solely from the perspective of environmental impacts. Bacenetti and Fiala (2015) evaluated the carbon emission footprints of five different AD plants by considering energy consumption and production through the LCA approach. The carbon emission footprints savings range from -0.208 to -1.07 kg CO_2eq kWh^{-1}, contributed by the substitution of energy production from fossil fuel. The outcome of LCA is dependent on the system boundaries and the chosen baseline scenario, which is difficult for cross-comparison for decision making. LCA is a systematic assessment tool, as described by Chang et al. (2011). The other limitation of LCA in evaluating waste to energy has also been discussed by Zhou et al. (2018), and several extension methods have been proposed for further development.

Leme and Seabra. (2014) conducted a comprehensive study, assessing the environmental and economic components of MSW. However, it has not been optimised simultaneously, and only single treatment approaches are considered at a time. Levis et al. (2014) formulated a generalised solid waste optimisation life-cycle framework to enable multi-period optimisation of solid waste management. One of the strengths of this framework is the design to be responsive to future changes in pricing, and the cost, environmental impacts as well as policy constraints are taken into consideration. Yang et al. (2015) developed an eco-efficiency analysis method aim to maximise the overall environmental improvement per unit investment cost in MSW processing. The eco-efficiency is estimated by dividing the environmental improvement by the economic cost of the measure (waste treatments). Roberts et al. (2018) present the implementation of existing solid waste infrastructure modelling system

(SWIMS) software in optimising the economic and environmental performance (environmental impacts, e.g. global warming potential) of waste management. SWIMS is a non-linear dynamic and LCA based optimisation tools. It is useful in identifying the future capacity requirement and optimum infrastructure solution to meet future waste flows. Comparatively fewer studies have conducted combined cost and environmental optimisation, mainly due to the uncertainty in combining multiple criteria. The aggregation of results from economic and environmental assessments can also result in the loss of valuable information (Soltani et al., 2017). Multicriteria assessment highly depends on the allocation of weighting factors as well as the local policy and interests of the stakeholders, as discussed by Arikan et al. (2017). A weighting system is unavoidable when different criteria need to be associated. The study by Mirdar Harijani et al. (2017) included an economic, environmental and social objective function in the proposed model of MSW management. However, the focus is only on the pre-treatment stage, i.e. recycling. Antonopoulos et al. (2014) applied ranked analytic hierarchy process method to rank the sustainability of MSW treatment alternatives. It is suggested that incineration with energy recovery provides the best performance due to the higher recovered energy, whereas the other two options (refuse-derived fuel and anaerobic digestion) provide fewer capital costs. An alternative to assigning weighting factors is expressing environmental impact as an externality cost (Ao, 2017). Kim and Jeong (2017) assessed the recovery options for industrial waste to achieve minimum economic and environmental costs. Vadenbo et al. (2014) proposed a multi-objective mixed-integer linear programming optimisation model for waste and resources management for industrial networks. The model combines material flow analysis and LCA. A set of Pareto efficient solutions assesses the trade-off between environmental and economic performance without relying on weighting prior to analysis. A selection can then be made from the set of Pareto solutions.

To summarise, current literature is focused on the assessment of various waste processing approaches. The studies that addressed systematic planning methodologies to support the regional planning of waste management systems is relatively less (Jia et al., 2018), particularly integrated regional planning. The assessment mainly from GHG emission perspective or based on environmental impacts. It deserves more development to consider additional environmental footprints. Most of the proposed decision models use mathematical optimisation or comparative analysis by LCA. Engineering methods and graphical tools, e.g. Process Integration, Pinch Analysis (Klemeš et al., 2018), and P-graph, which traditionally have not been linked to the circular economy, can form a technical foundation from which to embed sustainability and circular economy into system design.

2.4.1.1 Waste Flow and Management in the European Union

The role of waste management in the context of a circular economy transition has been highlighted in a report by the European Parliament (2017). The transformation needs of residual and by-products increase with urbanisation and population growth. It is a critical part of closing the loop. The cyclical waste to resources systems should also have the characteristic that the environmental impacts are work toward sustainability. EU has adopted binding targets on municipal waste with a common EU target of recycling at least 65 % of waste and send no more than 10 % to landfill by 2035 (European Parliament, 2017). The goal is for a total of 75 % of packaging to be recycled. In 2014, Austria, Belgium, Denmark, Germany, the Netherlands and Sweden sent virtually no municipal waste to landfill.

Figure 2.5 shows the condition of WMS in different EU countries. It should be taking note that the air emission performance assumes the waste portion for recycling is sent to the recycling plant and recycled. This needs further examination as there have been cases where the waste supposes for recycling are ended in other countries (e.g. in Asia). In term of the waste amount per capita, Denmark, Malta, Germany, and Luxembourg have the highest (Figure 2.5a). The country with the highest waste emission intensity (Figure 2.5c) is not necessary for the country, which has the highest absolute amount of waste (Figure 2.5a). Waste emission intensity in the unit of t CO_2eq/cap considered the waste amount, waste management efficiency (Figure 2.5b) and the population in accounting the GHG emission. Germany is one of the top ten countries with the high absolute amount of waste, but in tCO_2eq/cap it has the best performance, contributed by the lower waste generation per capita and WMS which capable in mitigating (negative value represents emission reduction) the footprint of waste. By using EU average performance as benchmarking, Figure 2.5a suggests the countries which should implement waste prevention/waste reduction as a strategy to reduce the emission from waste management. Figure 4b shows the countries with different waste treatment performance. It provides an insight on which countries should undergo treatment transition (switch to greener treatment option), waste trading (import and export activities based on treatment capacity, distance and treatment performance) and enhancing treatment efficiency. It is serving as a guideline in selecting the target countries for improvement. Table 2.5 shows the performance of EU-28 member states in 2012 against the EU circular economy package 2030 targets. The waste management practices vary between the EU countries.

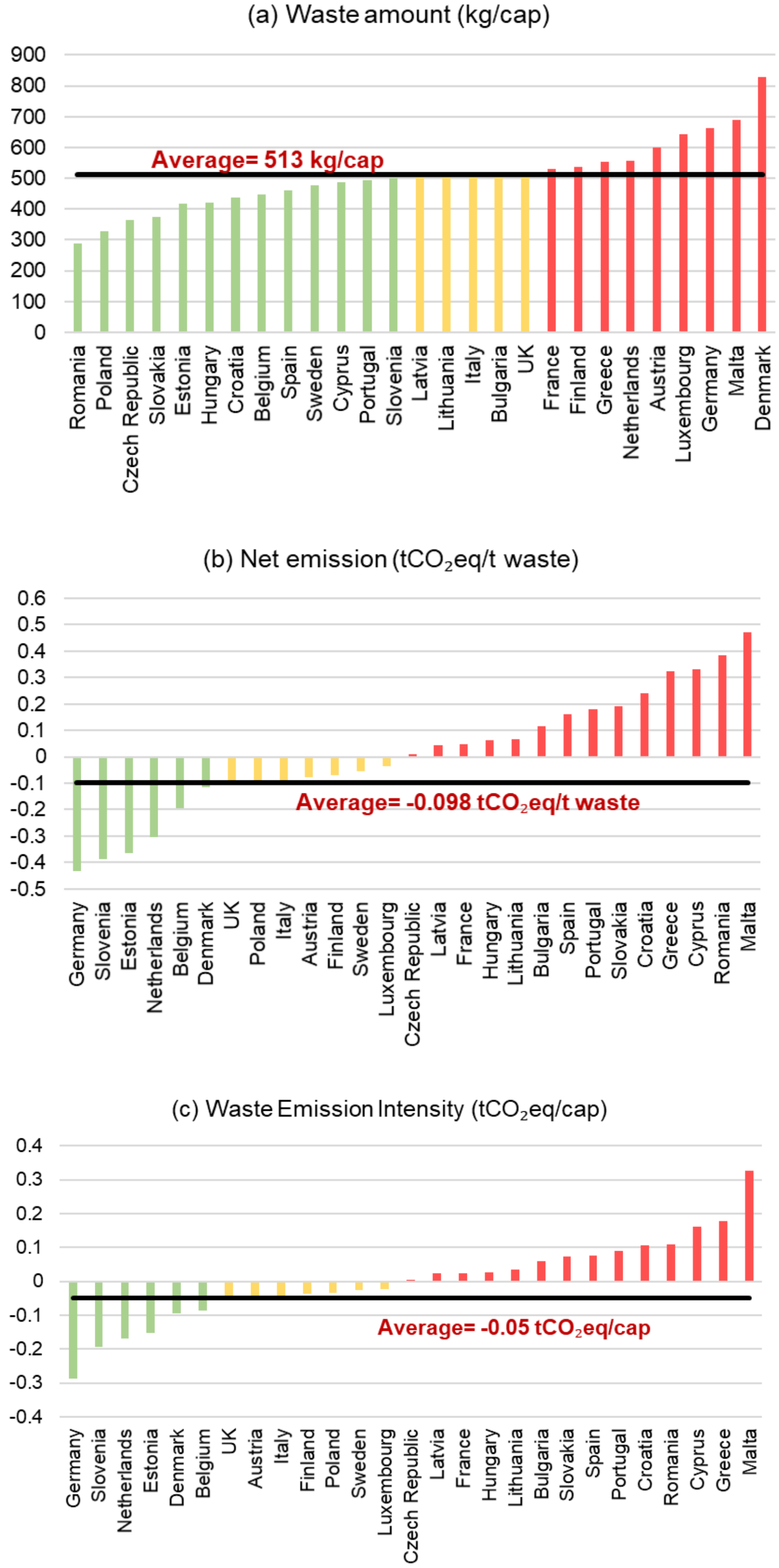


Figure 2.5: EU Business as usual statistics by using the 2030 waste amount projection a) waste amount b) net emission and c) waste emission intensity (Fan and Klemeš, 2019). Red = higher than average; Yellow = close to average or below 0. Green = lower than average

Table 2.5: Readiness of EU28 in achieving the circular economy package 2030 targets (European Parliament, 2017)

EU28	MSW		Packaging materials					
	<10% landfill	>65% recycle	Glass >85%	Metallic >85%	Paper & cardboard >85 %	Wood >75 %	Plastic >55 %	Total >75 %
AT	4.2 %	59.7 %	82.9 %	61.4 %	84.8 %	21.5 %	34.7 %	65.9 %
BE	1.0 %	56.2 %	100.0 %	97.3 %	89.8 %	66.1 %	41.5 %	80.3 %
BG	69.1 %	26.6 %	60.5 %	75.6 %	94.2 %	53.1 %	40.7 %	66.5 %
HR	82.6 %	15.1 %	62.8 %	12.5 %	96.1 %	0.4 %	45.4 %	59.7 %
CY	79.4 %	22.1 %	32.4 %	98.7 %	88.9 %	6.2 %	44.8 %	55.3 %
CZ	56.5 %	23.2 %	81.1 %	69.2 %	85.9 %	26.7 %	58.2 %	69.9 %
DK	2.1 %	41.0 %	80.6 %	51.8 %	76.5 %	40.4 %	29.4 %	60.1 %
EE	34.8 %	28.7 %	70.7 %	65.3 %	77.2 %	59.7 %	29.8 %	61.3 %
FI	32.9 %	33.3 %	77.6 %	85.3 %	99.2 %	16.9 %	25.4 %	59.3 %
FR	26.7 %	37.8 %	73.5 %	73.9 %	91.8 %	28.6 %	25.1 %	65.9 %
DE	0.2 %	65.2 %	84.7 %	92.3 %	87.6 %	30.3 %	49.5 %	71.3 %
EL	80.7 %	19.3 %	54.7 %	38.2 %	83.6 %	41.8 %	32.2 %	58.6 %
HU	65.4 %	25.5 %	34.2 %	80.8 %	73.0 %	18.1 %	27.8 %	48.5 %
IE	38.2 %	40.4 %	85.5 %	75.8 %	83.0 %	82.3 %	40.4 %	74.0 %
IT	39.1 %	40.0 %	70.9 %	73.6 %	84.5 %	54.2 %	37.5 %	66.6 %
LV	84.2 %	15.8 %	55.1 %	57.8 %	75.3 %	36.7 %	24.0 %	51.1 %
LT	73.0 %	24.3 %	72.2 %	67.2 %	82.4 %	48.8 %	38.9 %	62.2 %
LU	17.6 %	47.4 %	94.6 %	82.4 %	76.7 %	23.4 %	36.7 %	62.5 %
MT	82.2 %	12.8 %	21.3 %	41.5 %	77.2 %	0.8 %	32.8 %	46.6 %
NL	1.5 %	49.4 %	71.3 %	90.7 %	88.9 %	29.3 %	47.7 %	69.3 %
PL	59.2 %	24.8 %	51.2 %	46.9 %	53.1 %	28.5 %	22.2 %	41.4 %
PT	54.4 %	26.1 %	59.6 %	72.3 %	66.1%	69.7 %	30.4 5	56.9 %
RO	67.9 %	17.5 %	66.3 %	55.5%	69.8 %	41.1 %	51.3 %	56.8 %
SK	73.1 %	13.8 %	69.4 %	67.8 %	84.7 %	36.7 %	57.0 %	68.1 %
SL	42.5 %	48.8 %	87.3 %	41.6 %	78.7 %	33.1 %	64.8 %	66.9 %
ES	60.6 %	29.8 %	64.2 %	78.0 %	77.8 %	57.9 %	35.1 %	65.5 %
SE	0.6 %	47.2 %	88.2 %	74.4 %	76.8 %	17.2 %	34.9 %	56.9 %
UK	37.1 %	43.3 %	67.8 %	52.1 %	86.5 %	51.3 %	25.2 %	61.4 %
EU28	31.7 %	42.6 %	72.2 %	72.3 %	83.9 %	37.9 %	35.5 %	64.5 %

Austria (AT), Belgium (BE), Bulgaria (BG), Croatia (HR), Cyprus (CY), the Czech Republic (CZ), Denmark (DK), Estonia (EE), Finland (FI), France (FR), Germany (DE), Greece (EL), Hungary (HU), Ireland (IE), Italy (IT), Latvia (LV), Lithuania (LT), Luxembourg (LU), Malta (MT), Netherlands (NL), Poland (PL), Portugal (PT), Romania (RO), Slovakia (SK), Slovenia (SL), Spain (ES), Sweden (SE) and the United Kingdom (UK). Red = Far from target; Green =Target achieved; Yellow = Close to target

To summarise, regional level waste management planning could be a potential strategy to minimise the environmental footprints loops from material flow / waste management in the EU by sharing of resources, technologies, facilities and infrastructures. EU is an excellent candidate to perform regional waste management planning (case study) due to the established waste management policy and defined targets.

2.4.2 Transportation

Waste as resources is at no cost; however, the collection and processing could cost more than the value of the recovered product (e.g. biogas and digestate) (Jung et al., 2015). Travelled distance has been suggested as one of the main factors affecting sustainability. Numerous methodologies have been developed to support transportation planning. Transportation planning has been a wide scope problem, and it can be dealing with a variety of perspectives (government, economic, environmental, etc.). SteadieSeifi et al. (2014) divided the issues into strategic, tactical and operational planning problem with the following definition:

i. Strategic planning problems: investment decisions on the existing infrastructures (networks).
ii. Tactical planning problems: optimally utilising the given infrastructure by choosing services and associated transportation modes, allocating their capacities to orders, and planning their itineraries and frequency.
iii. Operational planning problem: Best choice of services and related transportation modes, best routes and allocation of resources to the demand. Real-time requirements of all multimodal operators, carriers and shippers. Deals with dynamicity and stochasticity that are not explicitly addressed at strategic and tactical levels.

There have been previous attempts in optimising waste collection and transportation. JUSTINE tool by Pavlas et al. (2017) offers simultaneous forecasting of the waste amount and waste parameters at different territorial units for a supply chain model. Ng et al. (2014) propose a supply network design with the optimal location of MSW processing hubs and facilities by multiple objectives optimisation models, where the economic and energy generation potential are demonstrated. An advanced tool, NERUDA (a logistics-based model) has been introduced by Šomplák et al. (2014) to support facility planning in the field of waste management, address logistic optimisation and capacity sizing. Optimisation of waste collection routes is vital to reduce the operating cost. Das and Bhattacharyya (2015) propose a scheme for the optimal waste routing between the transfer stations and processing plants of a city in India. The integrated SWM and the optimal path offer low emission and transportation cost. Similar studies were conducted by Malakahmad et al. (2014) in a city of Malaysia and Xue et al. (2015) in Singapore by using the geographical information system (GIS). Waste recovery technologies, together with localised management (collection route, collection system) minimised the burdening footprints of waste handling.

Varbanov et al. (2018) proposed a procedure for targeting the size of the WSM collection zone with the only consideration of GHG emissions as an environmental indicator. A computational approach has been suggested by Šomplák et al. (2019) to deal with the waste network flow problem. The newly developed approach was demonstrated through the example involving several producers for cost and GWP analysis. The average total processing cost in the subjected area was 74 EUR/t, and the average GWP was 37 kg CO_2eq/t. Vélazquez-Martínez et al. (2014) study the trade-off between cost and CO_2 emissions by using a multi-objective approach for the facility location problem. Hu et al. (2017) developed a bi-objective two-stage robust model to identify the strategies location (cost-effective, environmental-friendly) for the waste treatment facility. A comprehensive review was published by Bing et al. (2016) in assessing the operations research modelling methods for waste management and reverse logistics issues. The integration of operational research with other disciplines, e.g. LCA, can further facilitate a sustainable MSW recycling management.

The transportation-related consumption/footprint includes waste/feedstock collection and transportation, residue disposal, biogas and digestate distribution. WSM can be costly to transport compared to the value for recovered energy due to scattering throughout the city, high water content and weight. The MSW collection comprises most of the expenditure on waste management. It was reported that the collection costs could be up to 50 – 90 % of the MSW management budget (Das and Bhattacharyya, 2015). Rajendran et al. (2014) also highlighted that collection and transportation costs are the main factors in the profitability of the AD plant. Table 2.6 shows the estimated fuel consumption of the MSW collection and transportation operation in the urban and rural area. It should be noted that long-distance affects the feasibility of waste treatment options (e.g. AD) more than from the transportation cost and emission perspective. The transport duration also affects the energy content in the substrate as well as the biogas loss. Other than optimising the transportation network and allocation, enhancement of fuels and engine efficiency as well as introducing alternative energy source can also minimise the negative impacts of transporting.

Table 2.6. The energy input for collection and transportation of MSW, extracted from Pöschl et al. (2010).

Operation	Fuel consumption (MJ t_{DM} km^{-1})
Urban Area	
Collection	45
Transportation	3.9
Rural Area	
Collection	25
Transportation	3.9

Modal shift (change to a different transportation mode with different capacity, powered by different fuel types) is one of the measures that has received high research attention. Various decision models have been proposed to facilitate transport mode selection. De Paula and Marins (2018) applied a fuzzy logic approach, by having hamming distance, adequacy ratio and ordered weighted average operators as the algorithms, to assess subway, aeromovel system (an automated transit system), tramway and light rail transit. The environmental sustainability components are GHG emission, land utilisation and energy utilisation. Bandeira et al. (2018) develop a fuzzy multi-criteria model for the selection of sustainable urban freight distribution. They demonstrate the model by comparing the traditional intermodal distribution with the use of e-tricycles and propose a composite index to reconcile economic, environmental and social drivers. Environmental indicators include CO_2, NOx, PM, energy consumption as well as noise. Lam and Gu (2016) develop a bi-objective optimisation model to minimise cost and transit time with GHG emission as the constraint. Their results suggest barges as the transportation mode to be utilised whenever inland waterways are available and choose lorry as the transportation mode when transit time is the primary concern. Monte Carlo simulation (de Almeida Guinaraes et al., 2018) and adaptive neuro-fuzzy inference system (Al-Ghandoor, 2013) can also assess the sustainability of different modes of a passenger vehicle.

Operational research is vital in providing a set of decision-making tools, method and approaches for green transportation. Bektas et al. (2018) highlight the range of possibilities in dealing with green freight transportation that often goes beyond the remit of operational research. It should not be viewed as a one-size-fits-all (Bektas et al., 2018) remedy for all issues. There are different methods for analysing the modal shift in freight transport and its GHG reduction. The methods include choice modelling (micro), Semi LCA (macro), strategic freight transport network model (macro), decomposition analysis (macro), as well as hybrid methods (mix of micro and macro) (Jonkeren et al., 2019). Bouchery and Fransoo (2015) propose an optimal carbon emissions level of modal shift where exceeding this level could bring adverse impacts. Using transport cost and/or GHG emissions as the objective can lead to different internetwork designs. A similar concept is transportation mode shifting thresholds by Chen and Wang (2016) that derives from the analysis of different scenarios and CO_2 emission policies.

Although there has been a number of studies on transport selection, the considered scope and criteria differ from one another. Relatively few studies include non-GHG emissions and/or consider more than two transportation modes in a single study (Bask and Rajahonka, 2017). Fan et al. (2018a) show that the transport mode with the lowest GHG emission is not necessarily the best solution when considering other air pollutants. Most of the proposed decision models use mathematical optimisation, as summarised in Table 2.7.

Table 2.7: The transport mode selection studies with the consideration of environmental sustainability: Criteria and approaches

Ref.	Type of optimisation/ Assessment	Mode	Criteria							Environmental/ Green Criteria	
			C/P	T/S	Cap.	Freq.	Flex.	R	Q	Type	Quantification (Emission)
Hoen et al. (2014)	Inventory model	Air, road, rail, water	√	√						CO_2	Cost (Network for transport and environment method)
Zhang et al. (2013)	Bi-level programming	Road, rail, inland	√							CO_2	Cost (Range of prices)
Lam and Gu (2016)	Bi-objective optimisation model	Rail, truck, sea: Intermodal	√	√						CO_2	Amount (as constraint)
Le and Lee (2013)	MP model	Truck, ship, air: Multimodal	√	√						CO_2	Amount (EF-distance)
Liotta et al. (2015)	MILP model	Road, rail, sea: Multimodal	√	√	√					CO_2	Cost (EF-distance based on Ministry, French+ cost based on Government of Canada)
Regmi and Hanaoka (2015)	Stated preference methodology, mode choice model	Road, rail (Modal shift)	√	√				√		CO_2	Amount (EF-activity based)

Guo et al. (2016)	Evolution-strategy-based memetic Pareto optimisation model (multi-objective memetic optimisation approach)	18 transport modes with 3 different time	√	√						CO_2	Amount (EF fuel consumption)
Patterson et al. (2008)	Stated preference methodology, mode choice model	Rail and truck: Intermodal	√	√	√				√	CO_2	Amount, (EF distance & traffic estimates)
Kim and Wee (2014)	Semi. LCA, comparative analysis	Rail, truck, sea: Intermodal	√	√	√					CO_2	Amount (EF-distance)
Soysal et al. (2014)	Multi-objective LP	Road, sea: Multimodal	√	√						CO_2	Amount (EF-fuel consumption)
Macharis et al. (2015)	Combined multi-criteria decision analysis (AHP and PROMETHEE methods), GIS	Sea, road, rail: Unimodal, Intermodal	√	√				√	√	CO_2, noise hindrance	Amount (EF-distance)
Highlight the application/ Inclusion of GHG and/or air pollutants											
Qu et al. (2016)	Computational, Linear mixed integer program, Bi-criteria analysis	Truck, rail, sea: Intermodal, unimodal	√		√					GHG (Case study is CO_2)	Cost (EF-distance + cost based on World Bank)
Bauer et al. (2010)	Computational	Intermodal	√	√						GHG (Case study is CO_2)	Amount (EF-activity-based)
Corner et al. (2010)	The geospatial network optimisation model	Road, rail, sea	√	√	√					Emission (Case study is CO_2)	Amount (EF-activity based) least emission function etc
Yang et al. (2009)	Mobility Kaya Equation	Road, rail, sea, other subsectors								GHG	Amount (EF-energy consumption)
López-Navarro et al. (2014)	Comparative analysis (based on Marco Polo calculator)	Sea, road: Multimodal								CO_2 + air pollutants, noise etc	Amount (distance); External cost (Macro polo calculator).
Park et al. (2007)	Compare (emission impacts analysis)	Road, rail (Intermodal, unimodal)								Air pollutants	Amount (EF-activity based)

You et al. (2010)	Compare	Road, rail						Air pollutants (PM, NO_x)	Amount (EF-distance + Traffic simulation)
Lee (2011)	Compare	Road, rail						Air pollutants	Amount (Microscopic traffic models, no secondary pollutants)
Bickford et al. (2014)	3D Eulerian photochemical transport model (Community Multiscale Air Quality Model, CMAQ) + Weather Research and Forecasting Model (WRF)	Truck, rail (Modal shift)						Air pollutants	Emission impact (WIFE, Wisconsin Inventory of Freight Emissions)
Non-simultaneous assessment/optimisation (Environmental criterion is measured after the selection)									
Sunmi et al. (2004)	Logit models	Road, rail, sea: Multimodal	√	√				CO_2	Amount (EF-distance)
Márquez and Cantillo (2013)	Demand model	Road, rail, river	√	√		√	√	CO_2, air pollutants	Amount (EF-distance)
Li et al. (2007)	Time value model (mode choice)	Road, rail: Intermodal	√	√	√			CO_2	Amount (EF-distance)
Tao et al. (2017)	Stated preference methodology, RCL model	Road, rail: Multimodal	√	√				CO_2	Amount (EF-freight turnover, energy consumption per turnover)

EF = Emission Factor, C = Cost, P=Price, T = Time, S = Speed, Cap. = Capacity, Freq. = Frequency, Flex. = Flexibility, R = Reliability, Q = Quality, MP = Mathematical Programming, MILP = Mixed Integer Linear Programming, AHP = Analytic Hierarchy Process, PROMETHEE = Preference Ranking Organisation Method for Enrichment Evaluations

The collected papers in Table 2.7 (a total of 24) have been divided into three categories. The lead rows present the environmental criterion represented by CO_2 only, followed by the studies that consider other environmental issues (e.g. air pollutants) and finally the non-simultaneous assessment where the environmental criterion is measured after the selection. A few papers, such as López-Navarro (2014) highlighted that the integration of environmental issues into freight transportation planning is little explored. The review by Bask et al. (2017) states that the discussion on environmental sustainability with the other transport mode selection criteria is still a rather new and emerging topic. The environmental sustainability assessment is essential as the common assumption in freight transportation, such as 1) rail and vessel-based intermodal freight systems emit less CO_2 than truck-only freight systems (Kim and Van Wee, 2014), 2) sea transport is always preferable to road transport, 3) intermodal is always best in term of the environment (López-Navarro, 2014), are not always true.

Based on the collected studies in Table 2.7, the trend of defining the environmental criterion tends to be represented by CO_2 emissions, and in some cases, GHG. Different types of assessment methods are available and applied in the studies, which can basically be divided into two major approaches: cost-based or impact weighing. The emissions are either applying a price tag (e.g. MILP model by Liotta et al. (2015)), or the impact of different types of emissions are weighted (e.g. Stated preference methodology, mode choice model by Patterson et al. (2008)) for optimisation, See Table 2.7. Air pollutants are significant emissions of transport and are not always the co-benefit of CO_2/GHG mitigation strategies as discussed. Their exclusion in transport mode selection could lead to erroneous conclusions.

Studies based on a graphical approach for decision making is comparatively scarce. One such study proposes an iso-emission map (Vallejo-Pinto et al., 2019). The iso-emission map, based on the concept of isochrone curves, is useful to identify the suitable geographic scope for sea transport in relation to road transport in terms of GHG emission. Jonkeren et al. (2019) propose a shift-share components tool to visualise how changes in freight transport mode affect CO_2 emissions. In their graphical representation, the combination of the size and colour of bubbles from different transport modes communicate the extent that the shifting would contribute to CO_2 emission reduction. A graphical transportation decision tool has been presented by How et al. (2016) using weight/volume of materials to be transported and travelling distance as the two axes. However, their plot only compares two alternatives at a time, focusing on vehicle capacity constraints and CO_2 emission. Graphical-based decision-making tools primarily use the perspective of GHG emissions and deserve more development to consider additional emissions.

To summarise, exports/trading of recoverable and recyclable materials often view as waste pollution transfer and as a non-sustainable move. The collection and transportation distance are minimised (e.g. by optimising the collection route, transfer stations, plant location) in order to reduce the cost and environmental footprints. Sustainability can be achieved by waste trading, which considered that the region and countries could complement each other to develop a global circular economy. The compromise between a better treatment and a shorter transport distance on the net environmental footprints have to be assessed. Transporting activity creates burdening effect; however, if allocated adequately to suitable waste treatments (even in the other countries) and with the right transportation mode, the utilisation of the recovered products or utilities can create the unburdening effect on the overall system. The problem could be turned into an opportunity through trading for further emission reduction. An establishment of a fair-trading system and optimisation of waste circulation and utilisation across countries is the key. A decision support methodology is vital to ensure the sustainability of such trading, particularly to assess the collection and transportation activities. It should be noted that environmental consideration should not be limited to GHG emission. The limited inclusion of footprint could lead to footprint shifting. This is especially the case of transportation, as discussed by Fan et al. (2018a).

2.5 Process Integration and Pinch Analysis

Process Integration can be defined as a systematic and general method for designing an integrated production system ranging from individual processes to Total Sites and with particular emphasis on the efficient use of energy and reducing environmental effects (Klemeš, 2013). Pinch analysis is among the standard approach/technique for designing. Ho et al. (2017) stated that most of the identification of an optimal waste management strategy is performed by a "black box" mathematical optimisation approach. It is difficult to understand the reason for obtaining the optimal solutions fully. Pinch Analysis required minimum specific mathematical modelling knowledge. It originates from systematic efforts to improve heat recovery in the industry through process integration. Linnhoff et al. (1982) are the main pioneers of Heat Recovery Pinch in solving the Heat Integration problem. It offers a systematic thermodynamic based approach to address the need for large energy savings. This methodology has been widely applied to different fields and has the advantages to be easily understood. It is an effective targeting system engineering tool for supporting the system design. The impetus for solving energy-related issues has always been present as can be witnessed by analyses focused on specific industries such as steel, petroleum processing and economy-wide study. The conceptual and graphical techniques applied in Pinch Analysis have persisted even though mathematical programming techniques can also be used to resolve similar problems (Tan and Foo, 2007). This reflects the value of the intuitively appealing Pinch Methodology in solving real-life problems and for communicating results visually to stakeholders and decision-makers (Klemeš et al., 2018). The continuously evolving have stimulated the further development and expansion of the Pinch Methodology. Klemeš et al. (2018) divide the application to heat, exergy, renewable and waste heat, waste, hydrogen, power, water-energy, desalination, emergy (a measure of quality differences between different forms of energy), regional resources, and financial investment planning.

To summarise, PI has been a successful methodology in facilitating the network design toward sustainability (financial savings, energy savings, emission reduction, etc.). The graphical method allows the engineer to keep physical approach information of involved phenomenon compared to numerical optimisation techniques.

Tan and Foo (2007) developed an extension of Pinch Analysis as Carbon Emission Pinch Analysis (CEPA) for optimal allocation of energy sources based on the GHG emission constraints. CEPA is for macro scale regional planning; CO_2 emissions intensity is used as a quality index for energy flows. It has been a successful extension due to its capability to capture and communicate the challenge and opportunities in energy planning for low-GHG emissions. The carbon reduction target from the energy sector was set based on a national or regional development plan in CEPA; emissions reduction action is then decided to achieve the set target (Klemeš et al., 2018). There have been various studies applied CEPA for different energy system planning.

Crilly and Zhelev (2008) applied the CEPA to design the Irish electricity generation sector. TCEPA is proposed in the attempt to take account of the dynamic nature (time factor) of power demand and resources. This is especially for Ireland, which subjected to the inherent variability of renewable energies. Jia et al. (2009) adopted CEPA to identify the targets of minimum clean energy usage, energy demand and CO_2 emissions for a chemical industrial park. Atkins et al. (2010) extended the CEPA by considered the increased demand for electricity over a multi-year time horizon to analyse the electricity industry of New Zealand. It is suggested that the 90 % renewable target could be achieved by 2025 with careful planning. However, the economic merits need further assessment. Walmsley et al. (2014) modified CEPA by combining with energy return on investment (EROI) analysis to assess the feasibility of reaching and maintaining a renewable electricity target in New Zealand through to 2050. The suggestions toward low carbon emissions transport are the electrification of rail, uptake hybrid engine, introduction of biofuel and enhance the energy efficiency of a vehicle. Salman et al. (2019) applied CEPA for macro-level sectorial electricity planning in Nigeria. It was found that the minimum renewable target of 408 TWh is required to maintain the emissions level as in the year 2015 while meeting the projected demand of 530 TWh in 2035. Jia et al. (2016) proposed a multidimensional pinch analysis of the power generation sector in China, where carbon footprint, energy return on investment, water footprint, land footprint, and risk to humans are considered. Walmsley et al. (2015) adapted CEPA for transport energy planning with reduced GHG emission from freight and passenger transport. The considered emission reduction strategies include electrification, partial electrification and introduction of biofuels. The main components of the CEPA tool are CO_2eq emission as the y-axis, transport output (Mt·km) as the x-axis, the Demand Curve (purpose, mode, class of vehicle) and Supply Curve (fuels sources). The tool is mainly to identify and communicate how to achieve a fixed emission target. This approach has also been later applied to the case of Malaysia (Ramli et al., 2017).

In the study by Tan et al., (2018), CEPA is extended by combining it with Input-Output Analysis. This hybrid approach is applied to economy-wide analysis for the carbon-constrained economic growth of the Philippines. Pinch analysis-based methods have been increasingly used to carbon capture and sequestration since the development of CEPA framework, for example, recently by Thengane et al. (2019). The application of Pinch Analysis in waste treatment and management area is relatively limited. There are two studies proposed the Pinch approaches to the solid waste-related area: a) Biomass supply chain proposed by Lam et al. (2011) where the biomass supply chain, transportation and land use issues are tackle simultaneously and b) Waste Management Pinch Analysis (WAMPA) proposed by Ho et al. (2017). WAMPA was demonstrated by a hypothetical case study of five waste types. The strategies considered in the current WAMPA is limited, where only the treatment transition is discussed. The y-axis and x-axis of WAMPA are GHG emissions and waste amount. The absolute value could mask some of the critical information for an appropriate waste strategy planning, particularly if involving the net emissions accounting or comparison between countries. Another limitation of WAMPA lies at the assumptions of 3R activities have no emission, and WtE is given priority over 3R due to energy production and economic reasons. This does not truly reflect the real-life condition and is against the waste hierarchy. The WAMPA approach has been applied to a case study of China (Jia et al., 2018) using site-specific data.

To summarise, WAMPA which based on CEPA has a large potential for extension to facilitate the material/waste management planning at a regional level. The algorithms of WAMPA have to be improved in order to fit into the assessed problems and purposes. Most of the studies limited the environmental assessment to carbon emission footprint.

2.6 P-graph

P-graph (P-graph Studio, 2018) is a combinatorial optimisation framework for Process Network Synthesis (PNS) problems (Friedler et al., 1996). It was initially developed to solve problems in chemical process engineering where the cost-optimal structures and solutions, as well as near-optimal structures, are identified. The field of application has been expanded in recent years to at least 15 distinct applications, as reviewed by Klemeš and Varbanov (2015). P-Graph has proven useful in solving problems in supply chain management (Lam et al., 2010), discrete event decision making (e.g. evacuation plan by Garcia-Ojeda et al. (2012)), reaction pathways identification (Seo et al., 2001), and energy conversion (Aviso et al., 2017). Koing and Bertók (2019) recently demonstrated the application of P-graph to the synthesis of transportation networks, while Éles et al. (2019) focused on energy supply composition. Waste and resource management is a new potential area that can benefit from the further application of P-graph.

The approach of P-graph differs considerably from conventional generic optimisation methods. P-graphs implements a two-stage approach first identifying the set of feasible structures (within a given maximal structure) and then optimising the flows within a defined structure. The emphasis on a structural optimisation means P-graph offers a comprehensive search algorithm leading to robust solutions and faster computational speeds (Tan et al., 2014). This advantage arises from the two-stage approach in P-graph and can be seen in optimisation algorithms that apply the same two-stage methodology, e.g. (Walmsley et al., 2018a). However, the need to define a maximal structure, especially in the graphical-based P-graph Studio, limits the scope of possible problems that can be solved in P-graph. As a result of the structural optimisation step, the algorithms of P-graph enable the identification of both the optimal structure (and flows) and also many near-optimal structures (Aviso et al., 2017). The term "optimal solution" refers to the best possible solution identified by the P-graph Studio solver, which automatically converts graphical inputs to model parameters, variables, constraints, and an objective. The term "near-optimal solution" refers to other alternative structures (second-best solution, the third-best solution, and so on), which are less preferable compared to the optimal solution based on the given model. This is an important feature in dealing with waste management issues as it is difficult to capture in a mathematical model a high-fidelity representation of the real situation because of uncertainties, subjective parameters and weightings, and many practical constraints. The consideration of the near-optimal solutions provides more rational synthesis decisions. According to Walmsley et al. (2018b), the advantages of choosing P-graph over other mathematical programming tools are:

(i) The use of a graphical user interface for inputting maximal structures and displaying results

(ii) The emphasis on structural optimisation leading to optimal and near-optimal solutions, and

(iii) Software is open-source and provided free-of-charge.

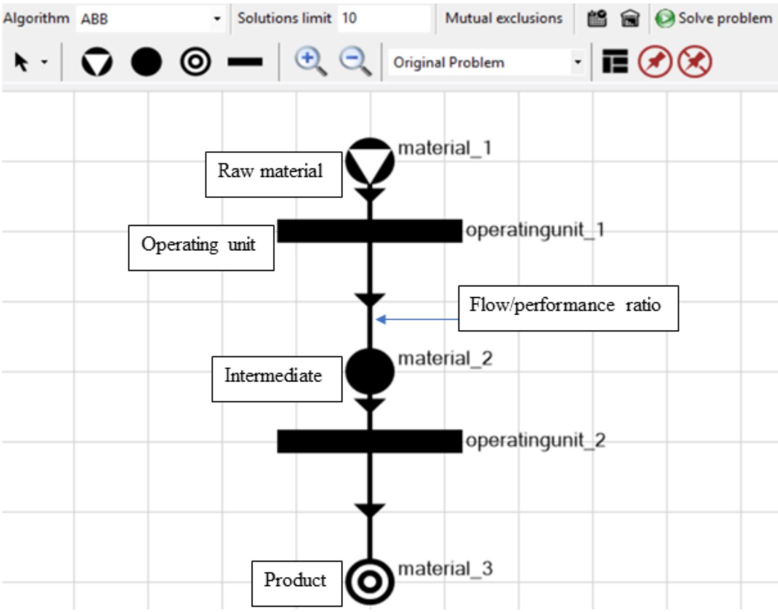


Figure 2.6: P-graph interface and the components. See Bertók and Heckl (2016) for detailed information on the structural representation.

P-graph is a combinatorial optimisation framework underpinned by five fundamental axioms (Friedler et al., 1992). These axioms give mathematically clear statements around the structural requirement of a problem. They are powerful in reducing the structural search space of optimisation to focus on analysing feasible structures. These are:

(i) Every demand (product) is represented in the structure,

(ii) A material represented in the structure is a resource (feed) if and only if it is not output from any operating unit (process) represented in the structure,

(iii) Every operating unit represented in the structure is defined in the synthesis problem,

(iv) Any operating unit represented in the structure has at least one directed path leading to a product, and

(v) If a material belongs to the structure, it must be input to or output from at least one operating unit represented in the structure.

P-graph Studio Version 5.2.1.10, (P-graph Studio, 2018) offers users the freedom to build maximal structures by connecting a series of vertices that represent flows and processes. It consists of five components: raw material, operating unit, intermediate, product and flow/performance ratio, as shown in Figure 2.6.

The latest development in P-graph Studio has been presented by Bertók and Bartos (2018) where the multi-period modelling can be accelerated. The design of multi-process MSW systems has the characteristics of a process network synthesis problem and, as a result, has been analysed for applicability to this vital area within the context of moving towards a CE. A proposed model is applied to vinyl chloride monomer production to avoid waste even during time periods when certain operating units are not available. To summarise, P-graph is a capable optimisation tool with several advantages as discussed. The application of P-graph is currently still limited, and its potential to solve a wide range of problem is still underexplored.

CHAPTER 3

BREAKEVEN BASED DECISION-MAKING TOOL FOR LOW EMISSION PLANNING

3.1. Application to Transportation Case Study

The work presented in this section is based on the author's publication in Renewable and Sustainable Energy Reviews entitled "Minimising the Energy Consumption and Environmental Burden of Freight Transport using a Novel Graphical Decision-Making Tool", as clarified on Page V (Contributing publication). The author of this thesis is the first and corresponding author of this publication. The other co-authors who contributed to this publication are the supervisor (J J Klemeš), co-supervisor (S Perry), and T Walmsley, where none of them is a student. My original contributions are listed in the introduction.

3.1.1 Introduction

The transportation sector heavily contributes to global energy consumption and resulting in air emissions. Recent studies by BP Energy (2018) project the transport demand will double by 2040 compared to that of 2016 in an evolutionary transition scenario. Air pollutants from transportation, mainly from the energy combustion, directly impact the environment and can also result in the formation of secondary pollutants, such as photochemical oxidants and secondary particulate matter, which can substantially harm human health. Traditional transportation issues (logistics/supply chain) are mainly managed from an economic perspective. Growing environmental awareness, however, has directed transportation towards environmentally sustainable options. The energy use and emissions highly depend on the technologies, fuels, vehicle operation, demand, demographics, road design etc. Available measures can be generally categorised into (1) energy efficiency improvement, (2) renewable energy and electrification, (3) transport mode optimisation, (4) public transportation, and (5) network relocation. Significant reductions require a combination of different reduction strategies (Bouman et al., 2017).

Modal shift is one of the measures that has received high research attention. Regmi and Hanaoko (2015) evaluated the shift from road to rail transport between Laos and Thailand by considering CO_2 emission. Tao et al. (2017) identified subsidies needed for shifting road to rail/water transport as a strategy to mitigate CO_2 emission. Boer and Essen (2011) summarised various studies endeavouring to estimate the potential shifting from the road and air transports to rail as well as the volume of goods physically suitable for the shift. Their literature review Boer and Essen (2011) suggests that the modal shift potential from the road to rail is 100 % for distances greater than 500 km, 40 % for 150-500 km and 5 % for 50-150 km. Kaack et al. (2018) summarise political targets of different countries, estimating the modal shift potential from the road to rail is between 4.1 to 50 %. For Korea, Hong et al. (2016) have determined reductions in the final energy demand by 25 % and GHG emission by 21 % are possible by 2020. Liu et al. (2018) identify a 36 % reduction in energy consumption for the transport mode optimisation scenario and a 32 % reduction in NO_x emissions. These results indicate that it is essential to identify the circumstances where the shift would be beneficial and sustainable. Transportation mode can be fuelled by different energy source (e.g. diesel, petrol, natural gas), including renewable fuel such as biodiesel. Different fuel types or energy sources contribute to a different level of the GHG and air pollutants emissions, depending on the fuel properties, processing technologies, and the resources at a place. Hydrogen and electrification have been one of the most studied energy alternatives of the recent studies. WRI (2019) stated that electrification does not make it equally suitable in all the places. There is no absolute answer on which transport mode is the best. The distance travelled, load to be transported, a model of the transport mode, as well as other concerns such as environmental and economic perspectives, frequency, reliability and speed, all influence the transport selection (Fan et al., 2018a).

Various decision models have been proposed to facilitate transport mode selection, but the considered scope and criteria differ from one another. Studies include non-GHG emissions and/or consider more than two transportation modes in a single study is relatively few (Bask and Rajahonka, 2017). The transport mode with the lowest GHG emission is not necessarily the best solution when considering other air pollutants. Most of the proposed decision models use mathematical optimisation. This study aims to propose a novel graphical approach to identify environmentally sustainable transportation modes. It facilitates the transportation selection by suggesting the mode with lower energy consumption, emissions and total environmental burden (TEB) for a given transportation distance and load. The applicability is demonstrated through a case study where three different kinds of transport modes (road, rail, sea) are considered. **My novel contributions include:**

(i) A new graphical tool where the ratio of the compared travelled distance (R) and load (L) is introduced to determine the selection with lower energy consumption and/or environmental burden (emissions).

(ii) A set of equations that forms the basis for the graphical tool, considering the transport load capacity and body weight of an empty vehicle. Marginal emissions are considered rather than the average emissions of load and body weight.

(iii) The determination of a TEB that considers GHG emission and air pollutants contributing to smog/haze formation through environmental prices, which aids the selection of the transport mode.

These contributions are demonstrated in a case study that expands the scope of included transportation modes. The other potential extension and application of the developed graphical tools in assessing the transportation modes fuelled by different energy sources are also demonstrated.

3.1.2 Method

Figure 3.1 shows the overall framework that underpins the graphical decision-making tools for transportation mode.

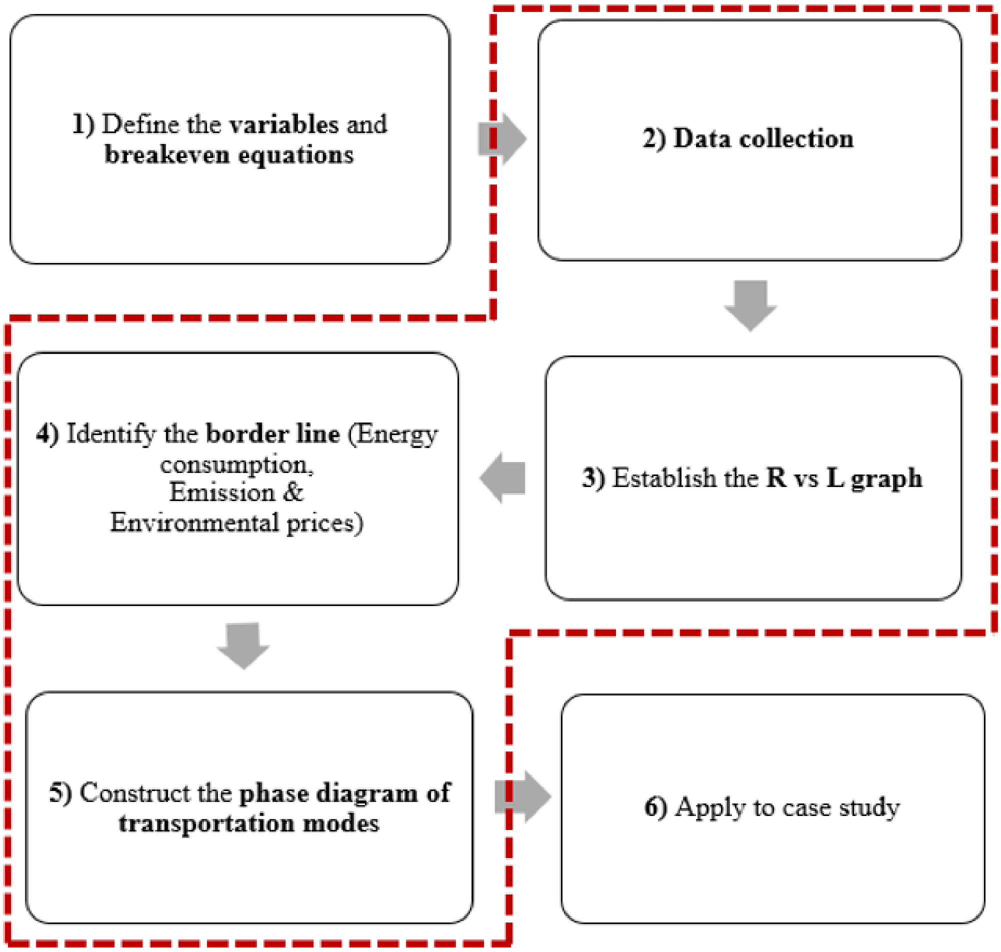


Figure 3.1: Overall framework in developing the graphical method for transport selection. R is the distance ratio; L represents a load.

The graphical tool can facilitate the rapid selection of transportation modes by considering energy consumption and environmental sustainability issues. The methods section is divided into two sub-sections. Section 3.1.2.1 describes the generic model, the considered variables and the breakeven equations that underpin the construction of the graphical decision-making tool. Section 3.1.2.2 demonstrates the construction of the graphical tool applied to the selection of freight transportation. The applicability is illustrated through a case study of transporting goods from Rotterdam to Antwerp and from Rotterdam to Genova. The case studies description and the data inputs are presented in Section 3.1.3.

3.1.2.1 Model Description

This section presents the generic equations to construct the graphical tool. The independent variable is the "breakeven" R-value (distance ratio of different transport modes). The breakeven point in this context defines when two transport modes would generate equivalent energy consumption and emissions or TEB.

Energy Use and Emissions

The total energy use or emissions released (E_{tot}) is determined using Eq(3.1). Eq(3.1) is formulated based on the idea that energy and emissions from a vehicle are linearly proportional to its total weight (body weight of empty vehicle + load). Most transport energy and emissions factors are reported for a fully-loaded vehicle on a per t of transport freight. As a result, the first term ($n\ e_{empty}\ D$) in Eq(3.1) relates to the energy or emissions due to the bodyweight and the second term ($L\ e_{load}\ D$) determines the energy or emissions due to the weight of the load.

$$E_{tot} = \left(n \cdot e_{empty} + L \cdot e_{load}\right)D, \quad \text{where} \quad n = \text{Roundup}\left(\frac{L}{w_{l,max}}\right) \quad \text{and} \quad n \in Z^{+} \tag{3.1}$$

Where e_{empty} is the specific energy use (or emission) of an empty transport vehicle fleet (MJ/km or t/km); e_{load} is the marginal specific energy use (or emission) of a transport vehicle fleet per t of transport load (MJ/tkm or g/tkm); n is the required number of transport vehicles; D is the total transport distance that each vehicle has to travel (km), and L is the total transport load across all vehicles (t).

Both e_{empty} and e_{load} are independent of L and D and can be related to standard full-load energy (or emission) factors, EF_{full}, which have the units of MJ/t·km (or g/t·km), noting t (in the denominator) is a ton of transport load (excludes the empty vehicle weight) and a transport distance in km.

$$e_{empty} = EF_{full}\left(w_{l,max} \frac{w_{empty}}{w_{full}} \right) \tag{3.2}$$

$$e_{load} = EF_{full}\left(\frac{w_{l,max}}{w_{full}} \right) \tag{3.3}$$

Where $w_{l,max}$ is the maximum load that one vehicle can transport (t), w_{empty} is the weight of an empty vehicle (t), and w_{full} is the weight of a full vehicle (t).

To identify the point where the energy use or generating emission of two transportation modes (i and j) are the same, i.e. $E_{tot(i)} = E_{tot(j)}$, the following equation has been obtained for the ratio R, which is D_i/D_j, for a constant L.

$$R = \frac{D_i}{D_j} = \frac{n_j \cdot e_{empty,j} + L \cdot e_{load,j}}{n_i \cdot e_{empty,i} + L \cdot e_{load,i}} \tag{3.4}$$

In the developed graphical tool, R is plotted on the y-axis, and L serves as the x-axis. To construct a breakeven line on the graphical tool, L is varied from 1 to 100,000 t. A log scale is applied to the axis. The identified border divides the space and suggests that under a given amount of load (L) to be transported and the known distance ratio of two routes (R), which transportation mode would have lower energy use or emission. Section 3.1.2.2 provides more details and a demonstration of constructing the graphical tool.

Total Environmental Burden (TEB)

The plot $E_{tot,i} = E_{tot,j}$ can only captures and compares a single dimension, e.g. one type of emission. TEB, T_{env} (€), as in Eq(3.5), is introduced to account for the emissions of both GHG and air pollutants by summing the cost/price contribution of each emission/pollutant, k.

$$T_{env} = \sum_{k} \left(E_{tot}(k) c_{env}(k) \right) \tag{3.5}$$

Where c_{env} is the cost coefficient (e.g. carbon tax, environmental prices) of the emission type (e.g. CO_2eq, SO_2, NO_x and PM) in €/t. In this study, the environmental prices are applied as presented in Section 3.1.2.2, Table 3.4.

To identify the border where the environmental price is the same, $T_{env,i} = T_{env,j}$, the following equation is obtained. The R ratio is determined under a constant load L.

$$R = \frac{D_i}{D_j} = \frac{\sum_k \left(\left(n_j \cdot e_{empty,j}(k) + L \cdot e_{load,j}(k)\right) c_{env}(k)\right)}{\sum_k \left(\left(n_i \cdot e_{empty,i}(k) + L \cdot e_{load,i}(k)\right) c_{env}(k)\right)} \tag{3.6}$$

3.1.2.2 Construction of the Novel Graphical Tool

Different types of freight transports can be included in constructing the graphical tool by following the model described in Section 2.1 and the generic construction steps described in this section. The generic algorithm/steps in constructing the graphical tool are discussed with the support of Figure 3.2 and 3.3 (generic examples). The graphical tool consists of R as the y-axis, L as the x-axis where the lines represent $E_{tot,i} = E_{tot,j}$ or $T_{env,i} = T_{env,j}$. The lines show the "break-even" conditions where two transportation modes use the same amount of energy or emit the same level of emissions. Figure 3.2 shows the generic example of a simplified problem where two transport modes (e.g. Mode A vs Mode B) are involved for selection. The line separated the space into two areas where the area below the line is assigned to Mode A, meaning that Mode A has a lower energy consumption or emission or TEB. This study considers, as the possible transport modes, light lorry, heavy lorry, electric train (container), diesel train (container), container and a general cargo ship.

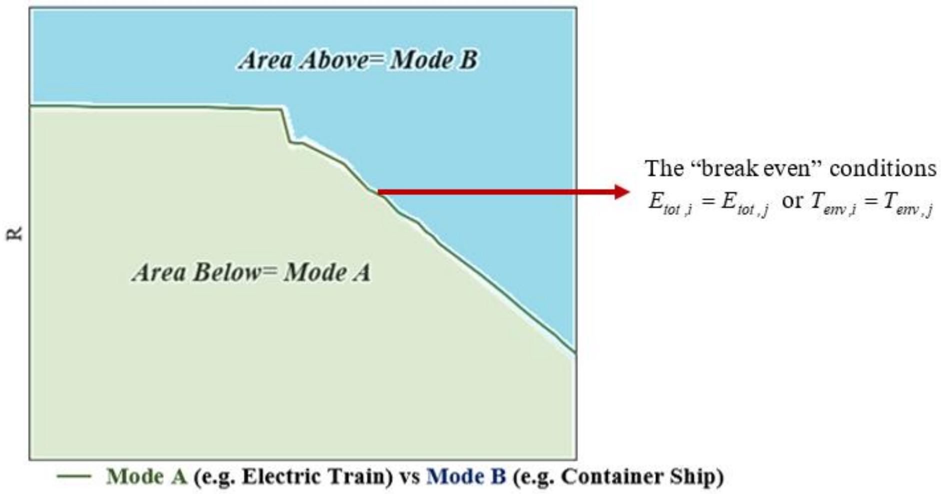


Figure 3.2: Generic example of a simplified problem: Selection between 2 transport modes

Figure 3.3 shows a more complex example where more than two transport modes are compared (e.g. four modes, consisting of four lines that represent the boundaries between different transport modes). The unnecessary lines can be eliminated to produce a defined space or area for transport modes with the lowest energy consumption or emissions. Elimination is based on the spatial relationships (e.g. encompasses, intersects, and/or overlaps).

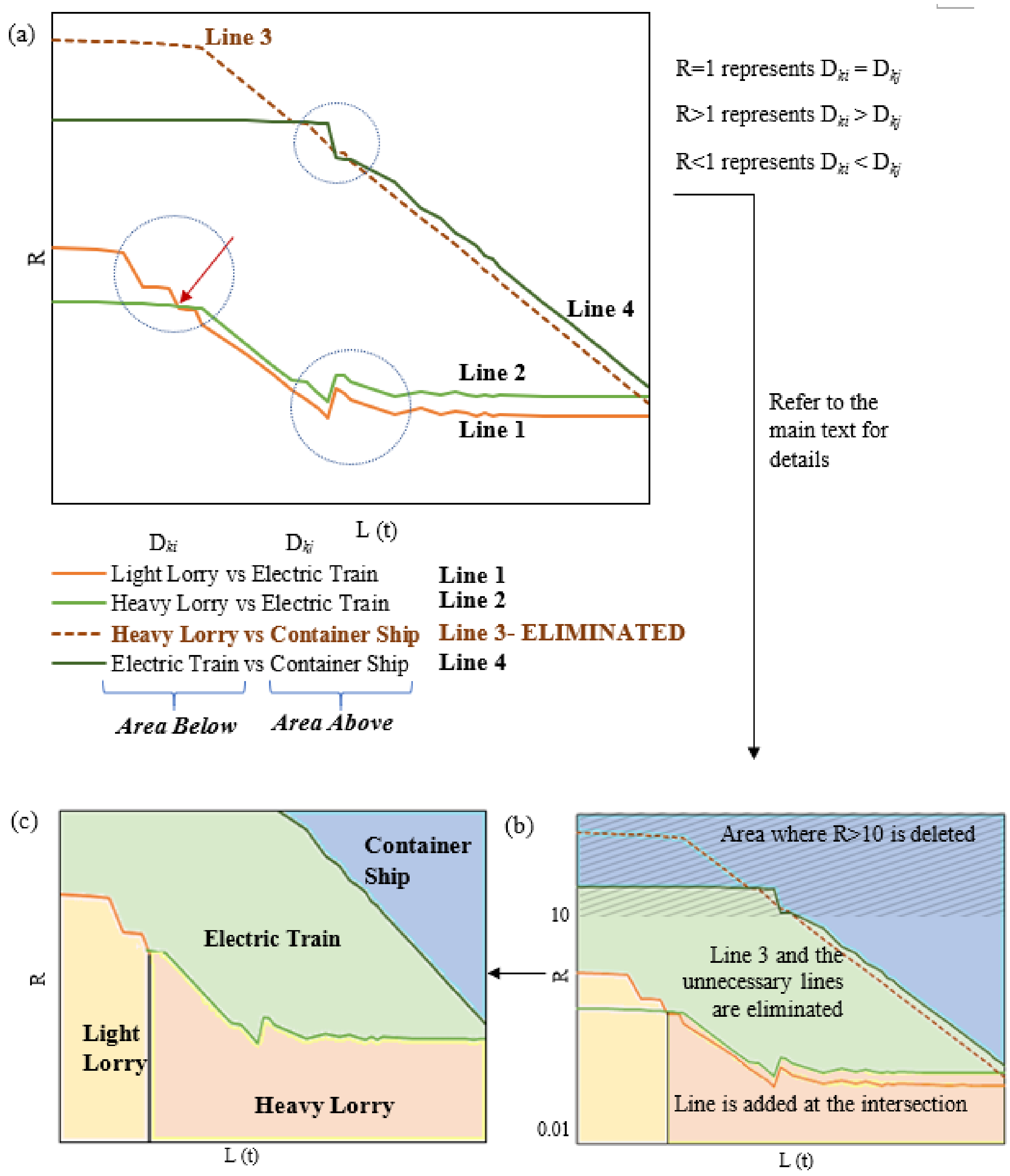


Figure 3.3: (a) Simplified illustrative example to explain the generic method of elimination, interpretation and the formation of graphical tools, supported by the discussion in the main text. Dotted circle represents the odd trends to be discussed. The dotted line represents the identified lines for elimination, see main text for the rules/algorithm. The examples of "elimination process" and "after elimination" are shown in Figure 3.3(b) and (c).

As demonstrated in Figure 3.3, the dotted brown line (Line 3) would be eliminated as the light green line 2, and dark green line 4 is the decisive/dominant lines. Line 3 shows that above the line is the area for a container ship. Line 4 also shows that above the line is the area for a container ship. Line 4 covers a broader area (overlap/ contains), and the compared transportation mode is an electric train. Line 3 shows that the area below the line is designated to the heavy lorry compared to shipping; however, lines 2 and 4 constrain the heavy lorry area to below the electric train. By following such described interpretation, Figure 3.3b is constructed in a way where the areas (under specific R and L) are designated to each transportation mode by colour code. To complete the graphical tools, (i) the line 3 and the other non-dominant lines are eliminated, (ii) the presented scale is adjusted by removing the area where $R>10$ and/or $R<0.1$ as the possibility of occurrence is very low, and (iii) a line is added at the intersection point. By referring to Figure 3.3c, there is an intersection point between line 1 in orange (i.e. light lorry vs electric train) and line 2 in light green (i.e. heavy lorry vs electric train). Both lines suggest the area above is designated to an electric train. At the left-hand side of the intersection point, line 1 is identified as the dominant line. The reason is that the area covered under line 1 is larger, which represents the circumstance when a light lorry is better than a heavy lorry. The area at the right-hand side of the intersection point of lines 1 and 2 are assigned to the heavy lorry. If the intersection point happened to be above the area of an electric train, the lower line would be the dominant lines as it covered more area of an electric train. Figure 3.3c shows the finalised graphical tool.

The rules can be summarised as:

(i) If mode A is compared to mode B, below the boundary line mode, A is preferred, and above mode, B is preferred.
(ii) If modes A and B (with common transport methods, e.g. road) are compared to mode C with R less than 1, the upper boundary is used, above which C is preferred and below which the mode (A or B) that drives the upper boundary is selected.
(iii) If mode A is compared to modes B and C (where B and C use a common transport method, e.g. sea) with R greater than 1, the lower boundary is used, below which A is preferred and above which the mode (B or C) that drives the lower boundary is selected.

Also, transport methods refer to road transportation, rail transportation and sea transportation. Mode refers to the sub-categories of transport methods, for example, light lorry, heavy lorry, electric train, diesel train, container ship and general cargo.

The graphical tool can be interpreted in a similar way as a phase diagram (Chemguide, 2014). A phase diagram is a graphical representation of the physical states of a substance under different conditions of temperature and pressure, where the lines represent the “phase” boundaries. In this transportation “phase diagram”, the boundary line represents the situation where both transportation modes have equal energy consumption/ emission. The distinct phase (area) represents the situation (*R* and *L*) where the listed transport mode has the lowest energy consumption/emissions in transporting the goods. By referring to Figure 3.3a, the dotted circle highlights the odd trends where there is a sudden increase, or decrease of R. These trends are contributed by the switch in a number of required vehicles (n_j and n_i) due to capacity limitations and the graphical resolution and representation on a log-log scaled plot. This algorithm is applied to a specific case as presented in the following discussions for Energy and for Emissions. The resulting graphical tool (with unnecessary lines removed is then applied to an illustrative case study in Section 3.1.3.

Energy

The energy use factors of each transportation mode are presented in Table 3.1. It is based on the vehicle specification reported by Boer et al. (2016). By inputting the data into Eq(3.4) and according to the description in Section 3.1.2.2, a graphical tool that compares different transport modes as pairs based on energy consumption can be constructed. The graphical tool shows all the “break-even” conditions (*R* and *L* values) where two transportation modes are utilising the same amount of energy. The occupied spaces represent the circumstance one of the transports have lower energy consumption.

Table 3.1: The maximum capacity and the energy utilisation of a full load vehicle (Boer et al., 2016)

Transport mode	Maximum capacity $w_{l,max}$ (t)	The energy use of a full-load vehicle EF_{full} (MJ/tkm)
Lorry, light <10 t	3	6.80
Lorry, heavy >10 t	13	3.30
Diesel Train (container)	288	0.37
Electric Train (container)	288	0.14
Ship (General Cargo)	7,339	0.22
Ship (Container)	54,160	0.22

Emissions

The evaluated emissions are GHG, NO_x, SO_x and PM. In this study, GHG refers to CO_2, CH_4 and N_2O, where CH_4 and N_2O are given a global warming potential of 28 and 265, expressed in CO_2eq (Boer et al., 2016). NO_x refers to mono-nitrogen oxides, e.g. NO, NO_2 and NO_3, which are expressed in NO_2eq. The data for maximum transport load, the weight of a fully-loaded vehicle, and the weight of an empty vehicle are presented in Table 3.2. The emission factors (g/tkm) of different transportation modes are presented in Table 3.3. The data inputs use the basis of a well-to-wheel life cycle (well to refining/generation, transmission, plug/pump to wheel), instead of tank-to-wheels (tailpipe only). Table 3.4 shows the environmental burden as a price for the different emissions. Environmental price expresses the loss of welfare/social marginal value due to one addition kg of pollutant being emitted to the environment, see CE Delft (2017) for detailed methodology. It has been widely applied to social cost-benefit analysis, corporate social responsibility and weighing in life cycle assessment. The estimation is based on the damage caused by environmental pollution or other such interventions with respect to a range of endpoint. Data listed in Table 9 to Table 11 include transport specification, emission factors and environmental prices are applied to the equations listed in Section 3.1.2.1.

The developed model based on the environmental price considered both GHG and air pollutant emissions in facilitating the decision making of freight transportation modes. It should be noted that the constructed graphical tool is based on the specification inputs reported by Boer et al. (2016), Table 9 – 11. The environmental prices (Table 3.4) are based on the context of the Netherlands. The environmental prices may differ between countries and changes over time due to differences in policy, local situation (e.g. population density) and concern. The inherent limitations and the sensitivity analyses are provided in CE Delft (2017). The presented case is mainly to demonstrate the construction and applicability of the proposed graphical tool. The data inputs can be substituted by transport modes with different specification and adjusted environmental prices for a customised model by following the generic model presented in Section 3.1.2.1.

Table 3.2: The capacity and weight of different transportation mode (Boer et al., 2016)

Transport mode	Maximum capacity (t), $w_{l,max}$	The weight of a fully-loaded vehicle (t), w_{full}	The weight of an empty vehicle (t), w_{empty}
Lorry, light <10 t	3	7.5	4.5
Lorry, heavy >10 t	13	28	15
Diesel Train (Container)	288	1,691	1,403
Electric Train (Container)	288	1,691	1,403
Ship (General Cargo)	7,339	10,000	2,661
Ship (Container)	4,060	20,000	15,940

Table 3.3: Emission factor of different transportation mode (Boer et al., 2016)

	Emission factors (EF_{full}), g/tkm			
Transport mode	GHG	NO_x	PM	SO_2
Lorry, light <10 t	634	0.7	0.078	5.5
Lorry, heavy >10 t	304	0.3	0.028	2.0
Diesel Train (Container)	35	0.373	0.011	0.035
Electric Train (Container)	19	0.017	0.001	0.01
Ship (General Cargo)	21	0.36	0.009	0.032
Ship (Container)	21	0.36	0.008	0.031

Table 3.4: The environmental prices (CE Delft, 2017), for the Netherlands

Emission	Environmental prices (€/t)
GHG (CO_2eq)	56.6
SO_x	24,900
PM	44,600
NO_x	34,700

3.1.3 Case Study

Two scenarios of transporting goods from Rotterdam (the Netherlands) to Antwerp (Belgium) and Rotterdam to Genova (Italy) help illustrate the application of the proposed tool in identifying the freight transportation mode with the lowest energy consumption or emissions. The mass goods to be transported are set in categories as 50 t, extended to 1,000 t for further discussion. Table 3.5 shows the travel distance for different transportation modes. Based on the information in Table 3.5, *R* values of different routes to the two destinations can be calculated. The freight transportation modes with the lowest energy consumption and emissions can be identified utilising the proposed graphical tool, with the *R* and *L* as feed in data.

Table 3.5: Travel distance of different transportation mode

Route	Distance (D), km	Reference
Rotterdam to Antwerp		
• Road ($D_{Antwerp}$ Road)	102	NTM (2019)
• Rail ($D_{Antwerp}$ Rail)	97	NTM (2019)
• Sea ($D_{Antwerp}$ Sea)	200	SeaRates LP (2019)
Rotterdam to Genova		
• Road (D_{Genova} Road)	1,182	NTM (2019)
• Rail (D_{Genova} Rail)	1,354	NTM (2019)
• Sea (D_{Genova} Sea)	4,093	SeaRates LP (2019)

3.1.4 Results and Discussion

The results and discussion section are structured in two sub-sections. The developed graphical tool is presented in Section 3.1.4.1 (for energy) and Section 3.1.4.2 (for emissions). The significant observation drawn from the models is pinpointed. Section 3.1.4.3 dealt with the case study. The environmentally sustainable transport modes (low energy consumption and low emission) of the studied case are suggested, followed by a discussion of potential tool improvement. Section 3.1.4.4 discusses the potential extension and application of the developed graphical tools. Tables 3.6 and 3.7 show the calculated value for e_{empty} and e_{load} based on Eq(3.2) and Eq(3.3). The values presented provides the base to facilitate the discussion and to understand the shares of vehicle and loads in weight distribution. In general, the bodyweight of a ship is higher than a lorry (Table 3.6), but the emissions and energy consumption factors of load are lower (Table 3.7) due to the larger capacity distributed among the load.

Table 3.6: Energy consumption and emission of the vehicle (e_{empty})

Transport mode	Energy MJ/km	GHG g/km	NO_x g/km	PM g/km	SO_2 g/km
Lorry, light <10 t	2.898	1,141.2	1.26	0.140	9.900
Lorry, heavy >10 t	7.856	2,117.1	2.09	0.195	13.929
Diesel Train (container)	88.411	8,363.2	89.13	2.628	8.363
Electric Train (container)	33.453	4,540.0	4.06	0.239	2.390
Ship (General Cargo)	511.662	41,011.1	703.05	17.576	62.493
Ship (Container)	478.901	67,952.2	1,164.90	25.887	100.310

Table 3.7: Emission factor of load (e_{load})

Transport mode	Energy MJ/tkm	GHG g/tkm	NO_x g/tkm	PM g/tkm	SO_2 g/tkm
Lorry, light <10 t	0.644	253.600	0.2800	0.0312	2.200
Lorry, heavy >10 t	0.524	141.143	0.1393	0.0130	0.929
Diesel Train (container)	0.063	5.961	0.0635	0.0019	0.0060
Electric Train (container)	0.024	3.236	0.0029	0.0002	0.0017
Ship (General Cargo)	0.192	15.412	0.2642	0.0066	0.0230
Ship (Container)	0.030	4.263	0.0730	0.0016	0.0063

3.1.4.1 Generic Graphical Decision-making Tool Development - Energy

Figure 3.4 shows the graphical tool results based on the energy consumption of different transportation modes under different loads and travelled distances. The train is the best option with the increasing load at R=1. This R-value is the condition for the transport routes having the same distance. The diesel train is not considered in the finalised graphical tools as the electric train is less energy-consuming than the diesel train under all circumstance. The case study assumes that the electric train is always available. The evaluation approach, if one of the options (e.g. electric train) not available, is discussed in Section 3.1.4.3.

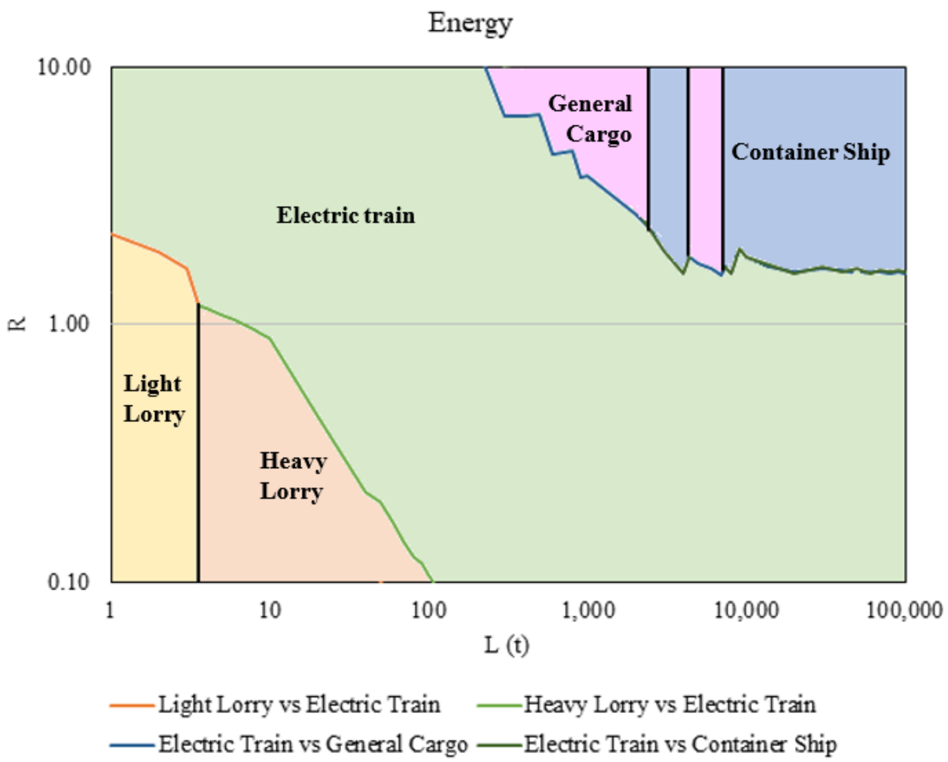


Figure 3.4: Graphical tool based on energy consumption.

An electric train has the lowest energy consumption per t of the load when the transported goods are more than approximately 10 t at R=1, as illustrated in Figure 3.4. The empty bodyweight of the train is heavier than a lorry, contributing to their high energy consumptions (see Table 3.6). However, their capacities are significantly larger such that the emission factor per t of load can be lower (see Table 3.7). The energy consumption per t of the load becomes lower than the lorry when it achieves the threshold. This consumption highlights the significant roles of the bodyweight of the vehicle when the amount of load is small. It is supported by the results published by Helms and Lambrecht (2007) in assessing the energy savings of different transport modes (road, rail, ferries and aircraft). They analyse the case when the empty weight of transport reduces by 100 kg. Light-weighting is a solution to reduce energy consumption in the use phase. Peng (2011) summarises the fuel consumption reduction potential of different technologies for the heavy-duty vehicle including aerodynamics, auxiliary loads, rolling resistance, mass/weight reduction, idle reduction and even intelligent vehicles. Weight reduction of empty vehicles can potentially reduce fuel use by 2 - 5 %. In a report of Directorate-General for Climate Action (RICARDO-AEA, 2015), an optimistic cost-effective weight reduction potential of up to 10 % by 2050 is proposed.

The energy consumption also largely depends on physical resistance – a function of the vehicle drag coefficient and velocity, which is especially true for road transport. Energy use can be higher than expected if operated in an urban area with regular stops and starts. The data input applied to build the graphical representation is based on average urban, rural and motorway transportation. Different data sets may result in slightly dissimilar trends. Other than physical resistance, different types and classes of transport modes have different engine efficiencies, body weights, and also energy consumptions. The specific data can apply to the generic model for a customised tool, e.g. for freight/logistics company, to facilitate the transport selection. The applicability is illustrated in Section 3.1.4.3.

3.1.4.2 Generic Graphical Decision-making Tool Development - Emissions

Figures 3.5(a) - (e) show the graphical tool results based on GHG, NO_x, PM, SO_2 and TEB. The boundary line represents the situation where both transportation modes have equal environmental performance. The distinct phase (area) represents the situation where the listed transport mode has a better environmental performance. The black line separates the space into two areas at the intersection, where the left side under the orange line belongs to the light lorry and the area under the green line is for the heavy lorry.

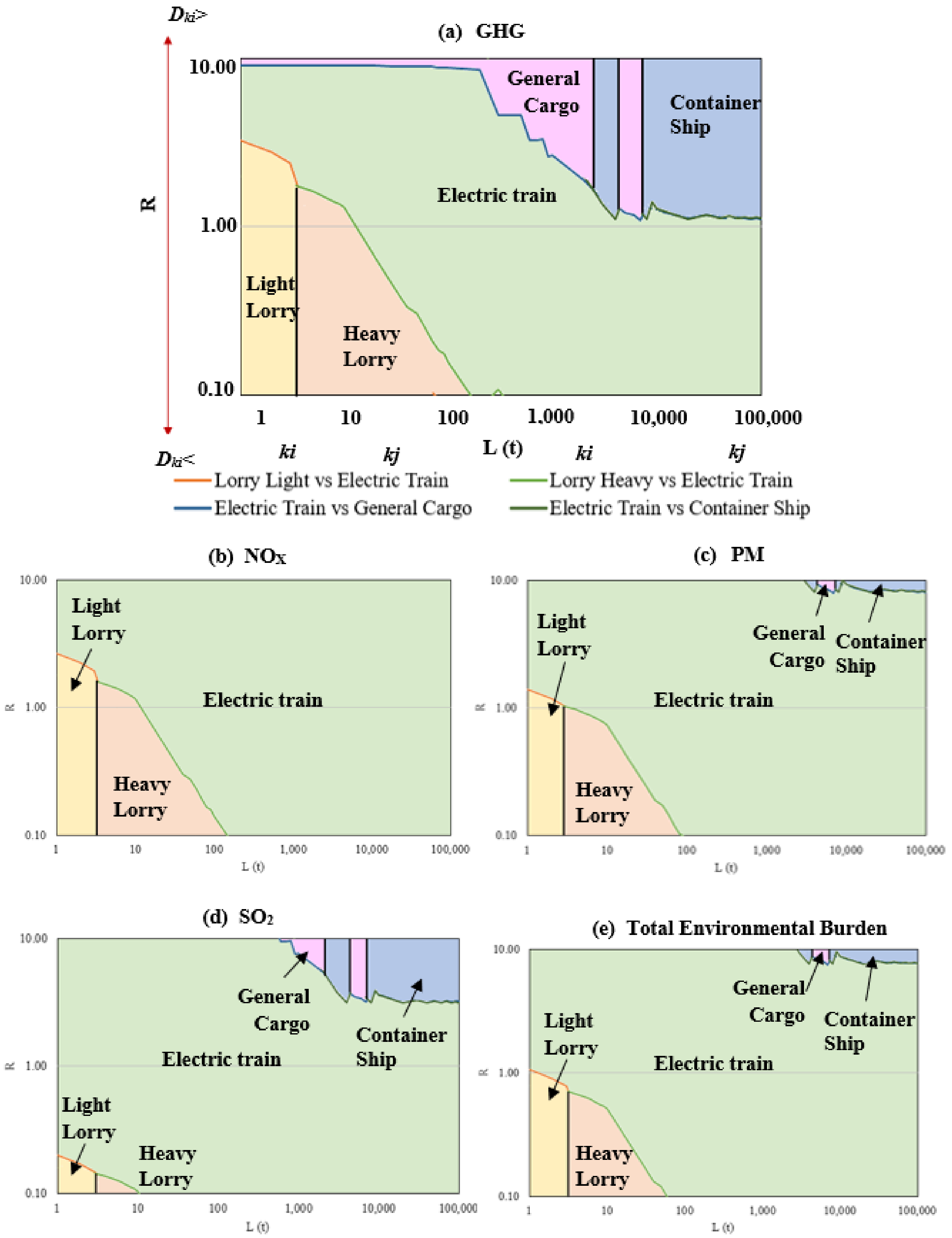


Figure 3.5: Graphical tool based on (a) GHG, (b) NOx, (c) PM, (d) SO_2, (e) TEB

Electric trains are the most environmentally friendly option in most cases, as observed by the larger area, especially when R=1. A lorry is a better option than the train only if the distance to travel by train (D_{kj}) is considerably longer, i.e. small R-value (D_{ki}/D_{kj}), and the load (L) is small as well. The train options are preferable with the increase of the load. When the train option is available, a ship (either container or cargo) would not be the preferred choice unless the route distance of the train is notably longer and/or the required load is very high. This trend is apparent, particularly for air pollutants emission (Figure 3.5(b)-(d)). The train is a better option under most of the circumstances (covered a larger area) in term of NO_x, PM and SO_2 emissions.

The graphical tool based on TEB (GHG, SO_2, NO_x, PM), Figure 3.5(e), highlights the role of non-GHG emissions could play in transportation selection. In Figure 3.5(a) (GHG), the general cargo or container ship is within the selection (have an assigned area), especially when the *L* is large. That is not the case in Figure 3.5(e) (TEB). The graphical area of sea transportation is small, suggesting that sea transportation is not recommended from the point of contribution in combined emissions (TEB) unless it is the only available method (e.g. shipping between islands/continents). The concern of environmental performance in decision-making has mainly focussed on GHG, such as studies on transporting wood pellet (Proskurina et al., 2016), aviation biofuel pathway (O'Connell et al., 2019), scenario analysis (Widyaparaga et al., 2017), emission of fuels (López et al., 2009), as GHG is subjected to the global agreement and the introduction of the carbon tax. The transportation modes with low GHG emissions sometimes have a higher emission of air pollutants. This can affect the overall selection of environmentally sustainable transportation mode and is even more complicated when it involves differences in route distances.

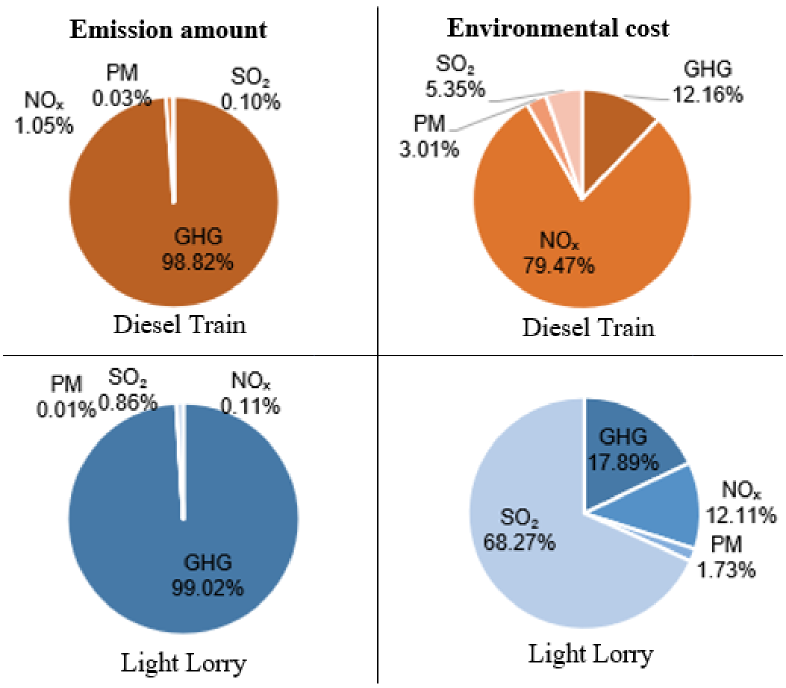


Figure 3.6: The contributions of GHG and non-GHG based on 1 t of goods and the same distance

Figure 3.6 illustrates in more details the roles of non-GHG emissions. The emission amount and total environmental price of transporting 1 t of goods under the same route distance are compared. By using the information in Table 3.3 and using light lorry and train diesel as an example, a contradicting trend in the emission amount and the total environmental prices can be observed. The pie charts show the share of emissions and environmental prices. GHG is the major emission by amount, constituting 99 % of the total emissions of a light lorry. However, the share decreases significantly when environmental prices are considered. SO_2 has the highest share (68.27 %) and is the dominant contributor to the environmental issue even when it has not been released in a high amount. A similar trend is observed in the case of the train (orange pie chart) as for the lorry (blue pie chart) where NOx is contributing to the high total environment price. The observed trend suggests that NO_x and SO_2 are the key emissions to be reduced in order to enhance the overall environmental sustainability.

3.1.4.3 Application of the Novel Graphical Decision-making Tool to Two Case Studies

According to the distance and route stated in Table 3.5, the R-values are identified as approximately:

- R-values of Rotterdam to Antwerp:
  a) D_{road}/D_{sea} = 0.5, b) D_{road}/D_{rail} = 1, and c) D_{rail}/D_{sea} = 0.5
- R-values of Rotterdam to Genova:
  a) D_{road}/D_{sea} = 0.25, b) D_{road}/D_{rail} = 1, and c) D_{rail}/D_{sea} = 0.25

Figure 3.7 shows that the electric train is the transport mode with the lowest GHG emission in transporting 50 t and 1,000 t of goods from Rotterdam to Antwerp and Genova by implementing the identified R-value. The electric train is the best option for both cases. The R values at the load of 50 t lie in the area of an electric train. Rail transportation has been reported by Bektas et al. (2018) as generally more environmental-friendly than road transportation. The total emissions in this study include those from energy consumption, i.e. the exhaust gas emissions (tank to wheel), the well to wheel life cycle emissions, as well as the contribution of wear and tear to emissions over time. The new graphical tool helps facilitate the selection of low emission transport modes. The same approach (as described using Figure 3.7) can be used to determine the best solution in terms of energy consumption, NO_x, PM, SO_2 and TEB (Figure 3.8). The identified best solution is an electric train for both cases, whenever an electric train option is available. However, it should take note that the results are applied to the electric mix described in Boer et al. (2016). Different results can be obtained according to the carbon intensity of a country, which is further discussed in Section 3.1.4.4.

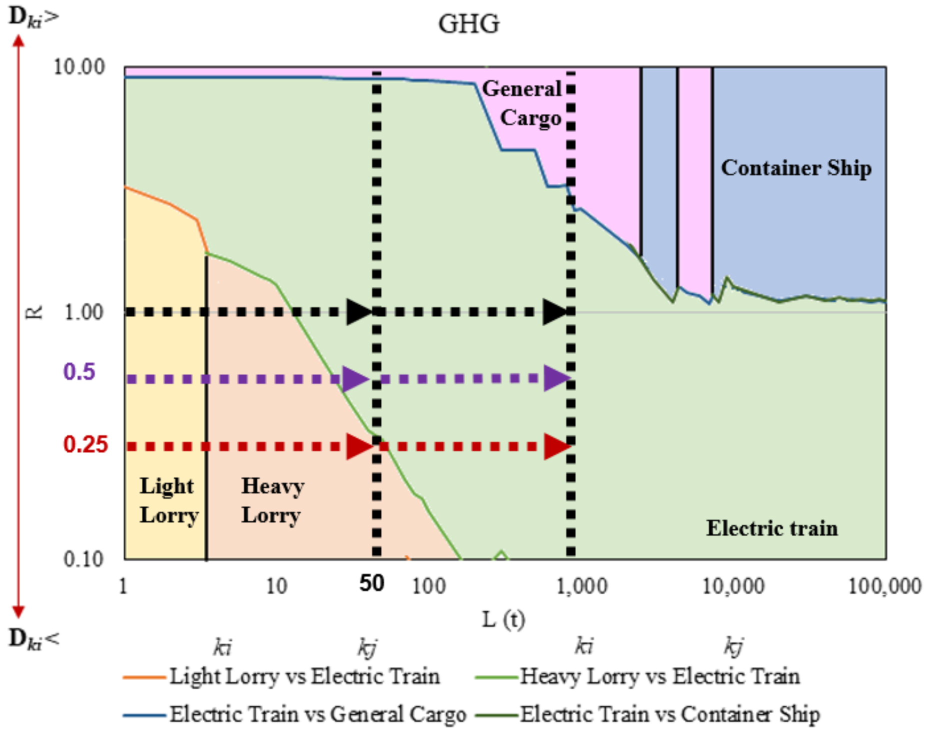


Figure 3.7: Graphical tool based on GHG emission - case study. Redline = Rotterdam to Antwerp; Purple line = Rotterdam to Genova

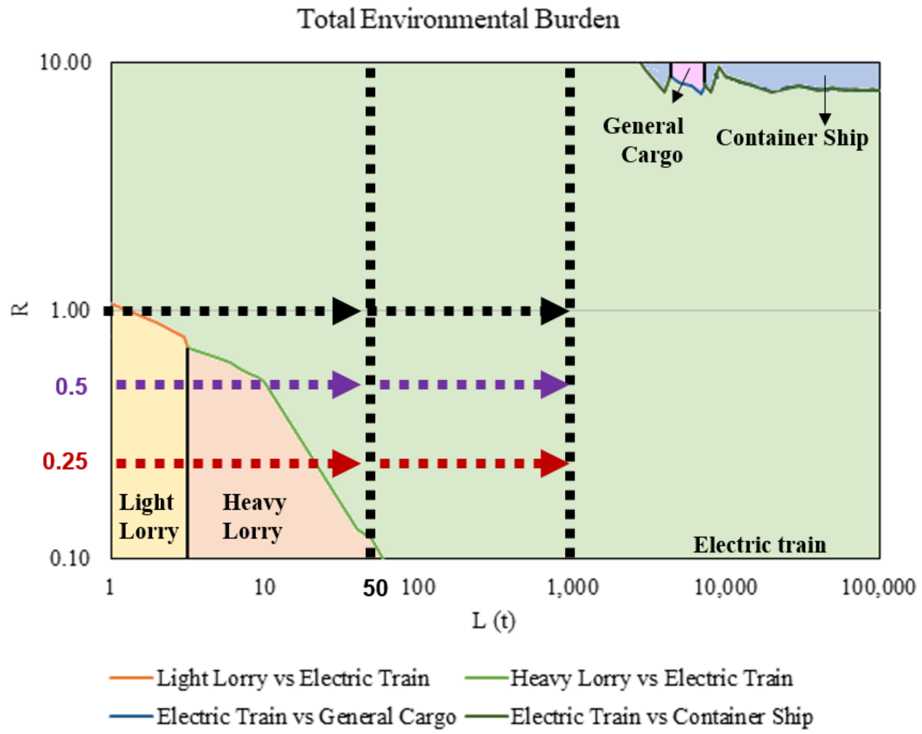


Figure 3.8: Graphical tool based on the TEB for the case study

The solutions presented are based on the full availability of all transport modes. An electric train is identified as the best solution for air emission (GHG and air pollutants) and energy consumption. However, there is the possibility that an electric train may not be an option. In this case, the graphical tool may be reconstructed based on the proposed method and a new set of graphs for the available transport modes. Figures 3.9 and 3.10 show two of the graphs that result from the situation without train availability. When the load to be transported is 50 t, the lorry is the preferred option for both transport scenarios. The ship (general cargo) emits less GHG pollution than a lorry when transporting a 1,000 t load. When considering TEB (Figure 3.10), the second-best options when there is no train possibility, the ship (general cargo nor container ship) is not chosen for loads under 50 t and 1,000 t. The result suggests that air pollutants from shipping are high, having a significant bearing on overall selection. The result highlights that the transport selection with the lowest GHG emissions (Figure 3.9, at 1,000 t Rotterdam to Antwerp = ship, see the purple dotted line) might not be the selection with lower air pollutants (Figure 3.10, at 1,000 t Rotterdam to Antwerp = lorry, see the purple dotted line).

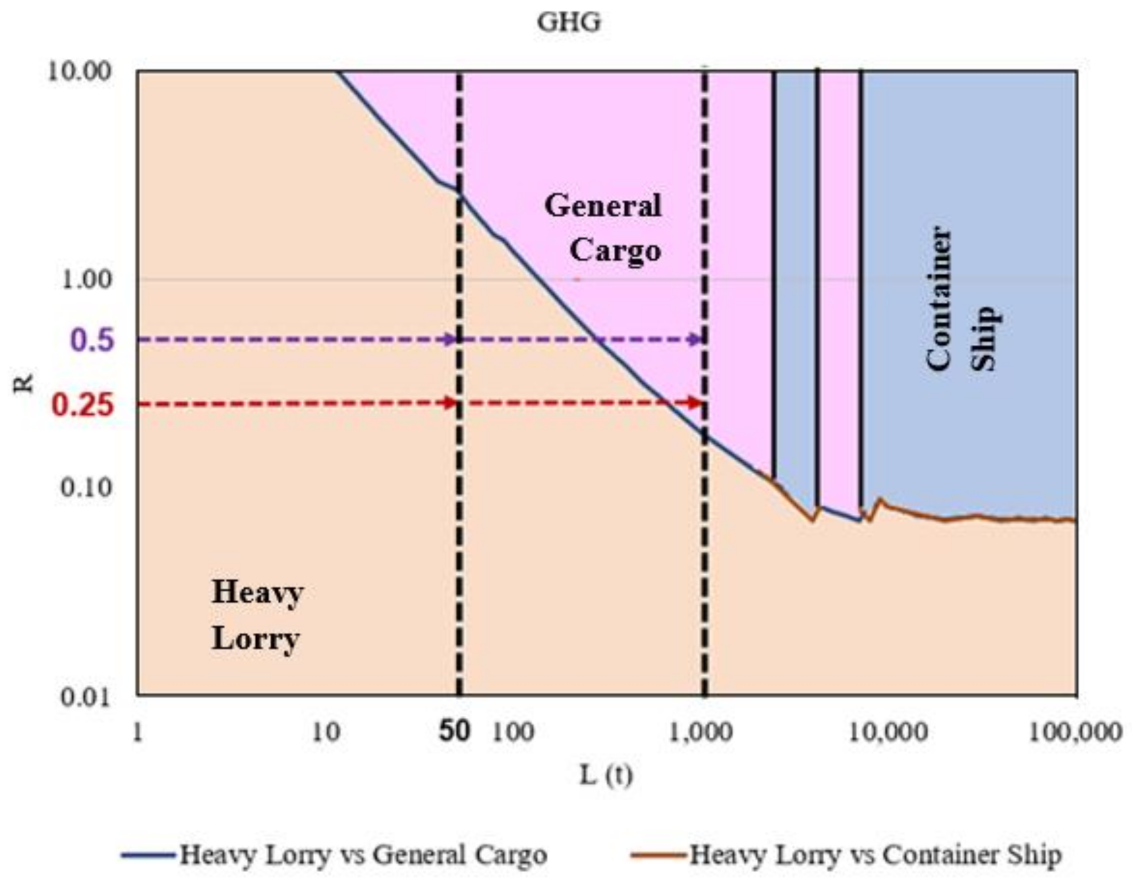


Figure 3.9: Graphical tool based on GHG emission (when is no train possibility)

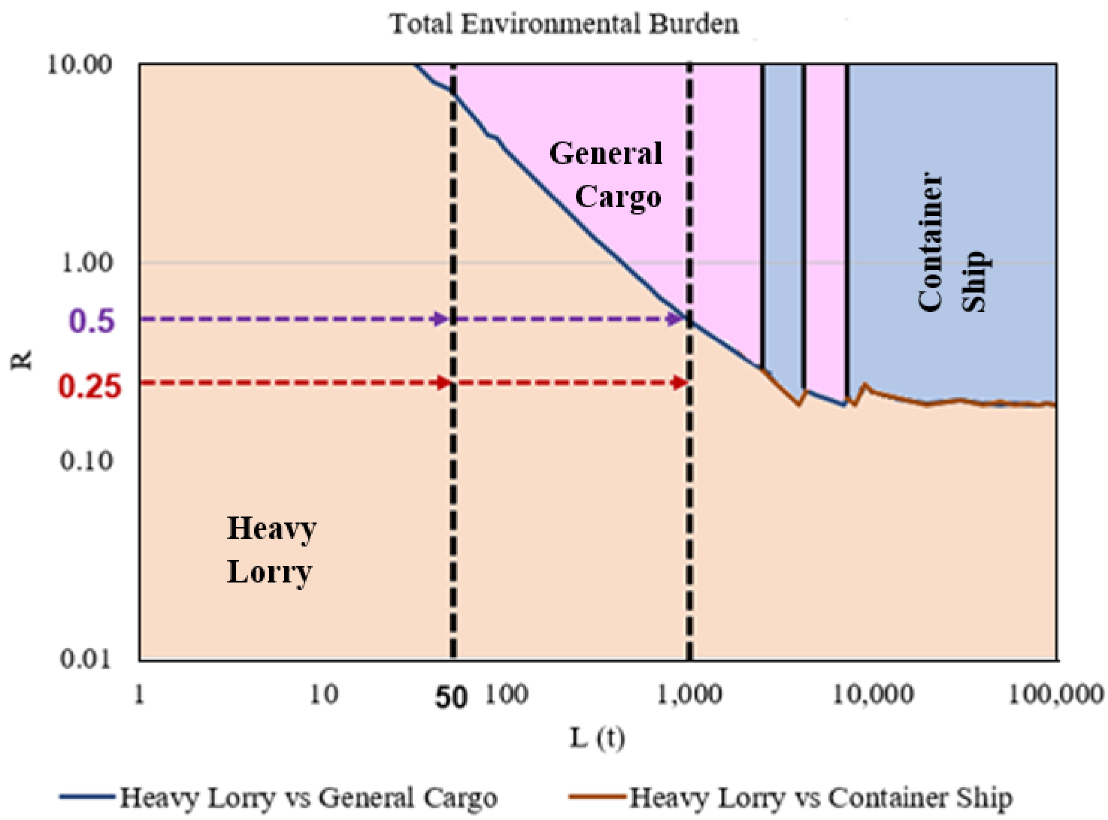


Figure 3.10: Graphical tool based on TEB (what if there is no train option)

3.1.4.4 Application to Different Countries and Possible Future Energy Mix for Transport

There can be many different types of fuels, engines, transport models and sizes which can result in the variances of emission and energy consumption per tkm. The comprehensive report by Boer et al. (2016) can be used as the fundamental source to extend this case study. To demonstrate the applicability, Figure 20 is constructed as an example to illustrate the impact of energy source (fuels type and electric mix (Fan et al., 2019b)). The energy sources considered for lorry are electricity, diesel, biodiesel, compressed natural gas (CNG) and liquefied natural gas (LNG). The emissions (GHG and TEB) of the lorry are compared to that of the electric train. The data is calculated based on the information reported by Boer et al. (2017), applying to the Eq(3.1)-(3.6) following the steps described in Section 3.1.2. Three scenarios are illustrated to show the impact of the electricity grid mix, considering the best, the worst and average:

i. Latvia, 1,168 g CO_2eq/kWh (Moro and Lonza, 2018) – the worst grid in the EU-28
ii. Sweden, 47 g CO_2eq/kWh (Moro and Lonza, 2018) – the best grid in the EU-28
iii. The EU 28 average, 447 g CO_2eq/kWh (Moro and Lonza, 2018)

Figure 3.11 shows the constructed graphical tool. It can be used to identify the low emission transportation with different energy sources when the load and travelled distance are defined. Figure 3.11(a)(c)(e) are for GHG and (b)(d)(f) for TEB. The graphs with coloured areas are the simplified version by keeping the best fuel type options for a lorry to compare with the electric train.

The following results have been identified:

i. In the case of Latvia (Figure 3.11a and b), at R=1 (distance to travel by lorry and train is equivalent), biodiesel lorry is the best from the view of GHG and CNG lorry by TEB under all assessed loads (1-100,000 t).
ii. A contradictory result is obtained in Figure 3.11(c) and (d). In Sweden, lorry run by electricity is the best from both GHG and TEB perspective. Sweden has a cleaner electricity mix than in Latvia. The electric train is the preferable option in Sweden with the increasing load. This is not in the case of Latvia, which dominated by biodiesel and CNG at R=1.
iii. At R=1, biodiesel is the option with the lowest GHG emission in EU-28 (Figure 3.11(e) and (f)). However, CNG is the best option when considering the TEB. This again emphasises the possible bias of considering only GHG emission in decision making. By referring to the zoomed view in Figure 3.11(f), it can see that the green line (Electric Lorry vs Electric Train) is very close to CNG. This observation suggests electrification generally leads to a lower TEB in EU for a country which has a carbon intensity of below average (447 g CO_2eq/kWh).

By referring to the identified value through the equations, taking L = 2,000, R = 1 as an example, the electric train is the selected options for Sweden as in Figure 20. It offers 30 % TEB reduction compared to the electric lorry option (1,660 € vs 504 €). Under the same condition (L=2,000 and R=1), CNG lorry offers 49 % TEB reduction (6,965 € vs 3,392 €) compared to the electric lorry. Based on the report by Eurostat (2018), 30 % electricity generated in EU is renewable sources; dominated by hydropower (36.9 %), followed by wind (31.8 %), solar (11.6 %) and others (e.g. wood, biogas, waste, geothermal). By countries, Sweden and Latvia have a share of renewable energy higher than the EU average. A contrasting result is obtained in this study where biodiesel and CNG are the preferable options than electrification in the view of GHG and TEB in Latvia. This is due to the methodology of emission accounting as the presented study is based on the Moro and Lonza (2018) where the import and export activities are considered. The electricity mix of Latvia is worsened due to the import from Estonia (GHG intensive source-peat). The emissions of an electric vehicle can be lower in the country dominant with non-renewable energy if the energy source is limited to renewable energy only (control system).

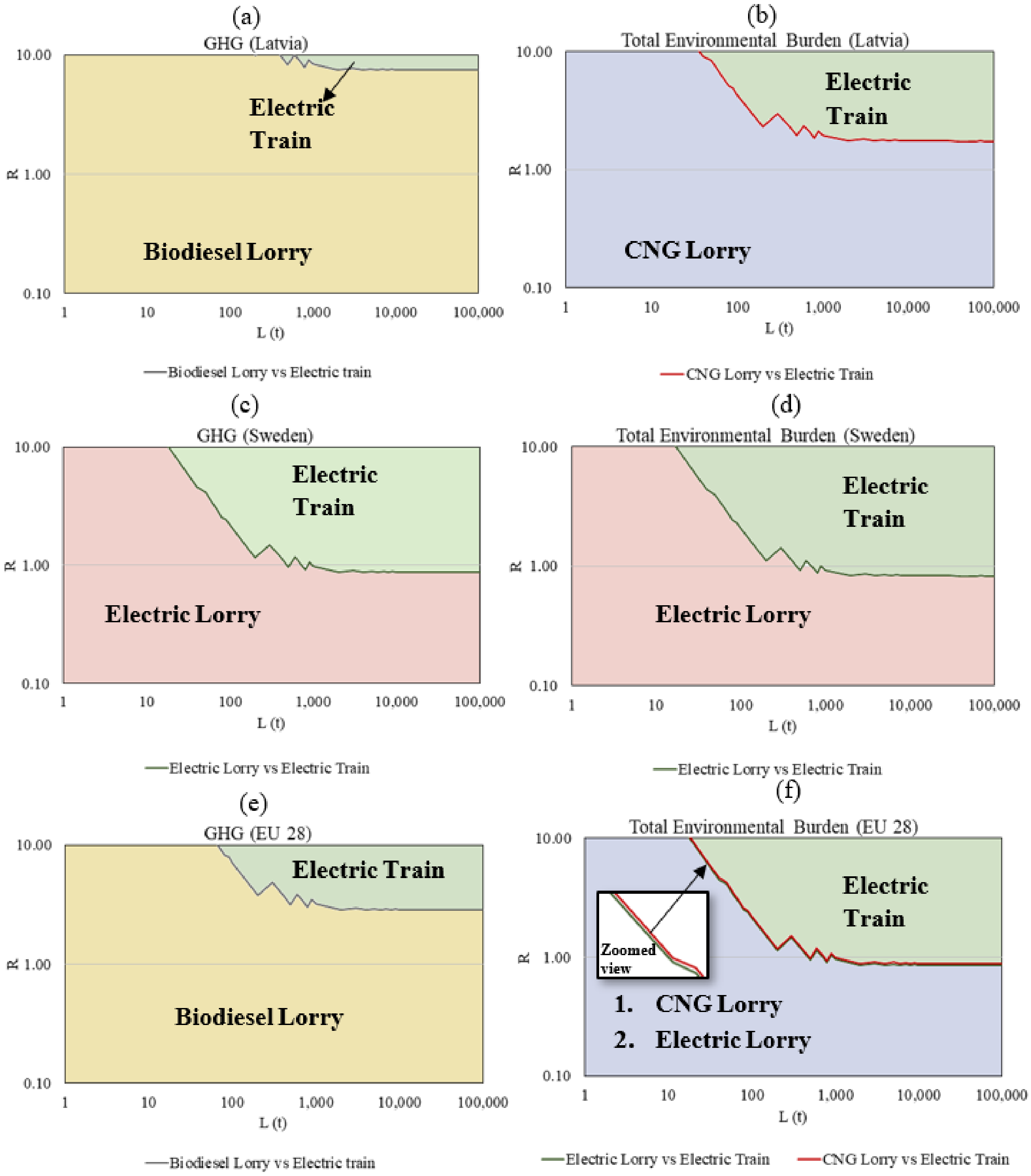


Figure 3.11: The graphical tool based on Latvia (a) GHG and (b) TEB; Sweden (c) GHG and (d) TEB; EU-28 (e) GHG and (f) TEB: EU-28. CNG= Compressed Natural Gas, LNG= Liquefied Natural Gas.

3.1.5 Directions for Future Research

The proposed graphical tool is environmentally oriented. The illustrated case study did not capture all the possibilities. However, the developed tool can be extended accordingly by using the equations and proposed algorithm as presented. The possible extensions and future studies include a) to consider a wider variety of decision-making criterion and b) apply to passengers' transportation, as elaborated in the following:

(a) Operational cost, frequency, flexibility and reliability are also an important criterion to be included in the decision making of the freight transport selection (Fan et al., 2018a). It can prevent the shift of footprints and reached a compromise between each criterion. The consideration of such factors is going to be a future study. Similar concept as the TEB model (GHG and air pollutants, see Figure 3.5(e), Eq(3.5) and Eq(3.6)) can be developed by using the sustainability index as a combined indicator of the multicriteria objective. Figure 3.12a shows the example of a composite graphical tool based on economic and environmental cost. The fuel price is based on IEA (2019) and energy content as in (The Engineering Toolbox, 2019), see supplementary information Table S1. The feasibility of the transportation (sea transportation and lorry) is enhanced when the economic aspect is considered (compare Figure 3.12a to Figure 3.12b).

This graphical tool is not included in the main findings. It is mainly to demonstrate the possibility of the mentioned extension. The economic value is only based on the fuel prices, which could vary across countries. The operating cost and taxes are excluded. A comprehensive economic oriented graphical tool integrated to the currently proposed environmentally-oriented graphical tool is the future study. Other than having all the criteria under an index, a contour plot can be constructed to replace the 2D graphical tool. This offers additional dimensions besides L and R.

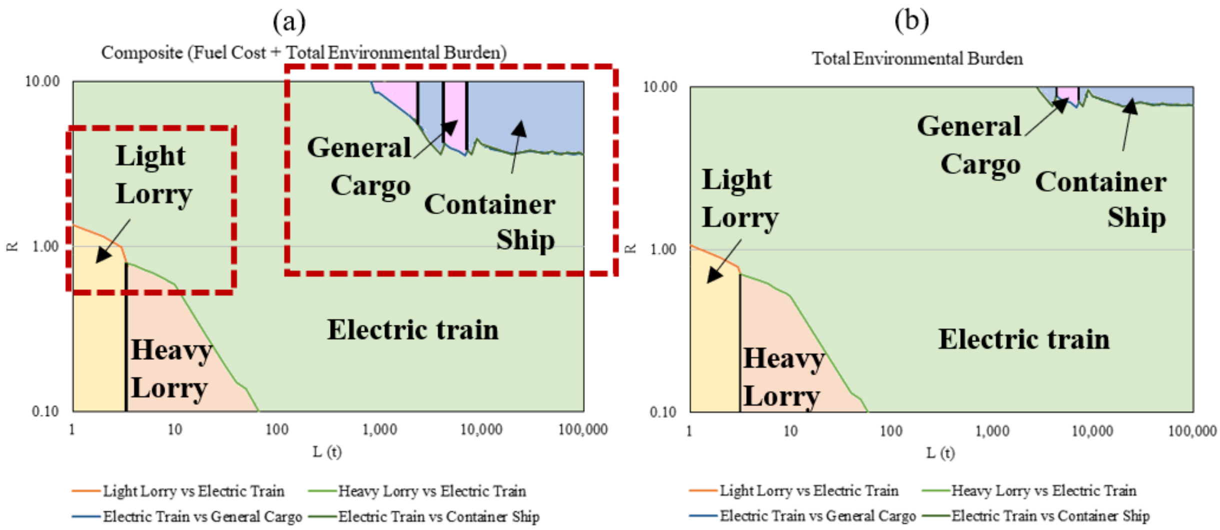


Figure 3.12: Graphical tool based on a) TEB and fuel price (Composite), b) TEB only.

(b) The proposed tool can also be applied to passenger transport by including electric car as one of the options. The model of electric cars with different efficiency and body weight can be the breakdown for a detailed assessment, as well as being compared to the other passenger transports run by petrol, diesel, compressed natural gas, liquefied petroleum gas, hydrogen and at different capacities. By extending the applicability of the graphical tools to tourist transportation (Hanpattanakit et al., 2018) can serve as a benchmark in setting the transportation fees toward the selection of a low emissions options. However, it should be noted that travelling time plays a significant part in deciding the selection of passenger transports and may not be the case in freight transports. The proposed graphical tools have to be improved by incorporating broader criteria and extended scopes.

Pinch Methodology (Klemeš et al., 2018) can be also be utilised in dealing with a more complex selecting situation/ transport planning in meeting the targets. The emission factors in constructing the graphical tool of this presented study considered the well to wheel cycle. The emissions from infrastructure (construction, maintenance) (Fridell et al., 2019) can be incorporated into the model for a more comprehensive insight in supporting the selection of freight transports.

3.1.6 Conclusion

The proposed model in this study can be used to determine the transportation modes with lower energy consumption as well as emissions for a particular load and travelled distance. The models which have been developed graphically are expected to ease the selection process compared to mathematical optimisation. The graphical tool is feasible for comparison of more than two transportation modes, and R is established as a way to prevent the model from being restricted to the origin-destination pairs considered. Environmental price is applied as a medium to consider both GHG and air pollutants (TEB), without which, it is inherently difficult to combine these due to the different environmental impacts. The results of the illustrative case study revealed that for transporting 50 t and 1,000 t of goods from Rotterdam to Antwerp and Rotterdam to Genova, the electric train is the freight transportation mode with lower energy consumption. An electric train is identified as the cleanest transport modes, in term of both individual emissions and TEB. However, this result can be varied according to the type of electric train and electricity mix of a country. By assuming an electric train is not available, under 50 t, the lorry is the alternative with lowest GHG; at 1,000 t, the ship is the better choice. The lorry is the better option when considering both GHG and air pollutants (TEB) in transporting 50 t and 1,000 t of goods. Sea transportation (General cargo or container ships) is preferable for loads of 10,000 to 100,000 t. Throughout the case study, two issues have been highlighted. (i) Bodyweight of transportation has a significant effect on the overall emissions and energy consumption. Together with focusing on engine and fuel efficiency, more effort should be diverted to develop lightweight vehicles. (ii) SO_2 and NO_x play a key role in the environmental sustainability of transportation. Low GHG selection is not equal to low air emission selection. Non-GHG emission causes more significant environmental impacts in transportation than GHG.

The proposed tool can also consider different fuel types and impacts of the grid mix. In demonstrating the extended applicability, the biodiesel lorry is found to be the best low GHG option for Latvia at R=1 (distance to travel by lorry and train is equivalent), regardless of the load. In Sweden, the electric lorry is the best from both GHG and TEB perspective while the electric train is preferable with increasing load. In the EU-28, biodiesel (renewable and biogenic) is the option with the lowest GHG emission, and CNG when considering the TEB. The importance of including air pollutants emission in sustainable transports decision making is highlighted. Electrification generally contributes to a lower TEB in the EU, especially for a country which has a carbon intensity of below average (447 g CO_2eq/kWh).

3.2 Application to Pyrolysis of Biomass

The work presented in this section is based on the author publication in Chemical Engineering Transactions entitled "Graphical Break-Even Based Decision-Making Tool to Minimise GHG Footprint of Biomass Utilisation Biochar by Pyrolysis", as clarified on Page V (Contributing publication). The author of this thesis is the first and corresponding author of this publication. The other co-authors who contributed to this publication are the supervisor (Prof Klemeš), Prof Raymond Tan and Dr Varbanov, where none of them is a student. My original contributions are listed in the introduction. My original contributions are listed in the introduction.

3.2.2 Introduction

The energy sector is one of the main contributors to GHG and air pollutants footprints. Various measures have been proposed or implemented to tackle this environmentally sustainable issues. The energy transition is one of the pathways toward emission mitigation by minimising the dependency on fossil energy. IRENA (2019) suggests the increased use of renewable energy combined with intensified electrification are decisive for the world to meet key climate goals by 2050. Energy from biomass (bioenergy) is one of the most investigated options. However, there is still an ongoing debate (Sterman et al., 2018) on carbon neutrality or renewable characteristics. Mitigation alone is deemed insufficient to achieve the Paris Agreement target in addressing the global warming/climate change issues (Haszeldine et al., 2018). Negative emission technologies (NETs) have to be deployed within physical and economic limits (Smith et al., 2016). Negative emissions can also be achieved by implementation biochar-based carbon management networks (Tan, 2019), besides the various emissions capture technologies, which have a relatively lower risk and investment cost. Pyrolysis is one of the notable pathways for biomass utilisation as the outputs are bioenergy and biochar with sequestration function.

The economic and emission accounting for a sustainable biomass utilisation remains a challenge in decision making due to its dynamic nature (the selection highly depends on the baseline scenario) and still subject to uncertainty (biochar application, biogenic carbon of biomass). Kulas et al. (2018) conducted the techno-economic analysis and life cycle assessment (LCA) of biochar as a soil amendment, as feedstock to produce activated carbon, and as fuel to displaced coal. Activated carbon is identified as the biochar utilisation that provides the highest mitigation benefits than as an energy source. Brown et al. (2011) assess the profitability of two biochar production, the value of biochar as a carbon offset plays a significant role; slow pyrolysis with the substrate cost of 83 USD/t is identified as not profitable. Yang et al. (2016) assessed the GHG emission of biomass-based pyrolysis in China and suggested the GHG intensity as 1.55 $x10^{-2}$ kg CO_2 eq./MJ. It is recommended that returning 41 % of biochar to the field would contribute to close to zero net GHG emissions. Fidel et al. (2019) studied GHG emissions when biochar ended on the soil. The differences in the results from laboratory incubation experiment and the impact of biochar at the field scale were highlighted as a pitfall.

A meta-analysis by He et al. (2017) suggests biochar application significantly increased soil CO_2 fluxes by 22 % but decrease N_2O fluxes by 31 %. The selection of the baseline scenario, the definition of displaced energy (avoided emissions) and the current understanding of biochar effectiveness and scalability needs to be further assessed for a consensus. The energy displacement is always done in reference to a baseline that needs to be clearly defined as the avoided emissions can change with the energy transition. There is an underlying assumption that the energy is being displaced (by energy with lower intensity). However, in some cases, the generated energy is fulfilling incremental energy demand. The complexity of the bioenergy system and its indirect effect, the selection of the system function and system boundaries that directly affect the results obtained have been highlighted by Lijó et al. (2019). Despite the inconsistent results, data that are changing from time to time according to the technology development, GHG intensity as well as the carbon tax (in this study, termed GHG price), a systematic methodology is a key to facilitate the decision making.

To summarise, there has been plenty of economic and environmental assessments on the pyrolysis processes of different biomass types and the biochar utilisation. The consistency of the decision-making methodology needs improvement, and it is generally based on scenario analysis. A systematic decision-making tool which considers the impacts under different circumstances, preferably in graphical form, with the capability of identifying the optimal biomass utilisation deserves further development.

This study aims to propose a graphical decision-making tool in facilitating the selection of biomass treatment or utilisation. **My novel contributions include:**

(i) A set of generic equations that form the basis for the decision-making tool, considering both the economic and life-cycle environmental footprint (in this case study GHG).

(ii) An extended graphical Break-even Based Decision-Making (BBDM) tool, where the environmental price (GHG) and the GHG intensity of energy are chosen to determine the suitable biomass utilisation. It is efficient in identifying the alternatives with the highest possible profit and lowest GHG emissions. The tool also enables the identification of suitable pricing to promote the treatment approaches.

(iii) A pyrolysis case study of biomass, where two types of substrates (a) energy crop and (b) agricultural residue for energy and biochar production, are assessed to demonstrate the applicability of BBDM. BBDM is designed to be feasible in capturing the optimal utilisation under the dynamic change of GHG price and GHG intensity of energy.

The developed BBDM tool is not limited to the presented case study, but for a broader range of decision making. A similar concept can be applied to the selection of environmentally sustainable transportation modes. The extended application is further discussed in the conclusion.

3.2.2 Method

This section presents the break-even relations that underpin the graphical decision-making tool as well as the algorithms for the construction. The break-even point in this context defines when two pyrolysis/biomass treatment processes (i and j) would generate equivalent profit, see Eq(3.7). GHG price is applied in order to identify a compromise solution for an economic-environmental decision as well as to reduce the multi-objective problem into a single objective. The total profit is defined as in Eq(3.8), $Profit_{economic}$ considers the earning from the selling of recovered products (energy and biochar) deducted by the operating cost of the entire life cycle, Eq(3.9). $Profit_{environment}$, defined in Eq(3.10), considers the GHG credit from recovering the energy and applying the biochar to the soil (sequestration) deducted by the emission released along with the processes which incur a penalty cost of GHG. Eqs(3.11) - Eq(3.13) show the estimation of GHG credit and GHG penalty incurred by the process. The independent variable is the "break-even" GHG price. Eq(8) shows the estimation of GHG price when the total profit of two pyrolysis processes are equal.

$$Profit_{total\ (i)} = Profit_{total\ (j)} \tag{3.7}$$

$$Profit_{total} = Profit_{economic} + Profit_{environment} \tag{3.8}$$

$$Profit_{economic} = Eenergy + Ebiochar - OC \tag{3.9}$$

Where $Eenergy$ are the earnings from recovered energy, $Ebiochar$ are the earnings from biochar, and OC is the operating cost.

$$Profit_{environment} = Cenergy + Cbiochar - P_{op} \tag{3.10}$$

$$Cenergy = AmountRE \times CI \times GHG_{price} \tag{3.11}$$

$$Cbiochar = AmountB \times SF \times GHG_{price} \tag{3.12}$$

$$P_{op} = A_s \times O_{ef} \times GHG_{price} \tag{3.13}$$

Where $Cenergy$ is the GHG credit from the recovered energy, $Cbiochar$ is the GHG credit from the application of biochar, P_{op} is the GHG penalty by the operating process, $AmountRE$ is the amount of recovered or generated energy (syngas, bio-oil and or biochar) by the pyrolysis process of agricultural waste or energy crops, CI is the GHG intensity of energy (e.g. electricity power) where the emission is associated with electricity generation from identified regions based on the energy mix, GHG_{price} = is the cost coefficient (e.g. carbon emission tax, environmental price), $AmountB$ is the amount of biochar produced, SF is the carbon emission sequestration factor of biochar, A_s is the amount of substrate, O_{ef} is the emission factor of pyrolysis processes. Eq(8) is applied to identify the break-even point/ boundary, where $Profit_{total\,(i)} = Profit_{total\,(j)}$. GHG_{price} is identified by varying the CI.

$$GHG_{price} = \frac{Eenergy_j + Ebiochar_j - OC_j - Eenergy_i - Ebiochar_i + OC_i}{AmountRE_i \times CI - P_{op,i} + AmountB_i \times SF - AmountRE_j \times CI - P_{op,j} + AmountB_j \times SF} \tag{3.14}$$

The generic steps to construct the graphical decision tool BBDM are as follows:

(i) Define the functional unit (can be based on carbon content, amount, e.g. 1 t or 1 ha of the substrate)

(ii) Define the assessed scenarios (e.g. different pyrolysis setting, type of substrate, the ratio of recovered products), system boundary and assumptions.

(iii) Collect the required data.

(iv) Define replaceable energy (Optional). $AmountRE$ in Eq(3.11) is equal to the replaceable energy if the recovered/generated energy from pyrolysis are all to displace the current energy generation practice. In some cases, the recovered energy is used to fulfil the increasing energy demand where the current energy generation practice (e.g. fossil fuel) is not being replaced. In this case, there is none or only a partial avoidance/unburdening emission ($AmountRE \times CI$).

(v) Apply the data to the Eq(3.14) to identify the GHG price.

(vi) GHG price is plotted on the y-axis, and GHG intensity of electricity serves as the x-axis. A graph of the reciprocal function ($y = \frac{1}{x}$ or $y = -\frac{1}{x}$) is obtained, see Figure 3.13.

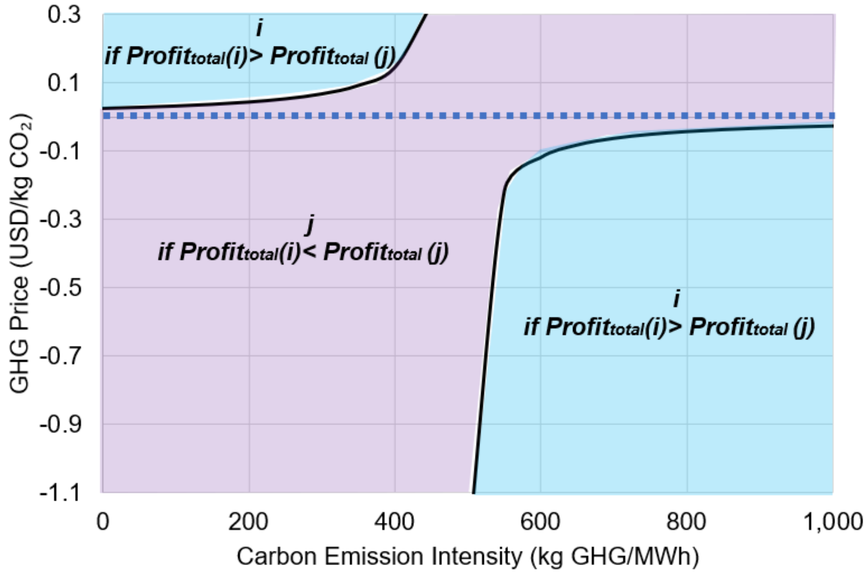


Figure 3.13: Generic example of the decision-making tool BBDM

(vii) Assign the area (label and colour). The identified border/line divides the space and suggests that under a given GHG intensity and the known GHG price, which is the scenario with the highest total profit (economic and environmentally). Figure 3.13 shows a generic example of the decision-making tool. The blue area is assigned to Case *i*, suggests Case *i* provided a high profit and lower emission than Case *j* in the blue area. The presented scale is adjusted by removing the area where GHG price < 0 (below the blue dotted line in Figure 1) as the GHG price is always ≥0.

3.2.3 Case Study

Figure 3.14 shows the overall framework of the case study. The type of substrates/biomass, assessed in this study, are energy crops and agricultural residues. The selected treatment option is pyrolysis, specifically slow pyrolysis system. The emission released during the field operation, including the use of fertiliser for energy crops are considered in this case study. Table 3.8 presents the assessed scenarios. The functional unit applied in this case study is 1 ha of the substrate (switchgrass or wheat straw). Table 3.9 shows the applied data. This study assumes all the recovered energy is qualified to replace the conventional energy generation rather than use to fulfil the increasing demand which is not eligible for avoided/unburdening emission accounting, see Section 3.2.2 Step iv. The second assumption is that there is available land which is suitable for biochar application. It should be noted that the graphical tool of this case study is based on the specification inputs reported by Gaunt and Lehmann (2008). In practice, localised data inputs are required to feed into the proposed methodology for a customised graphical tool and solutions.

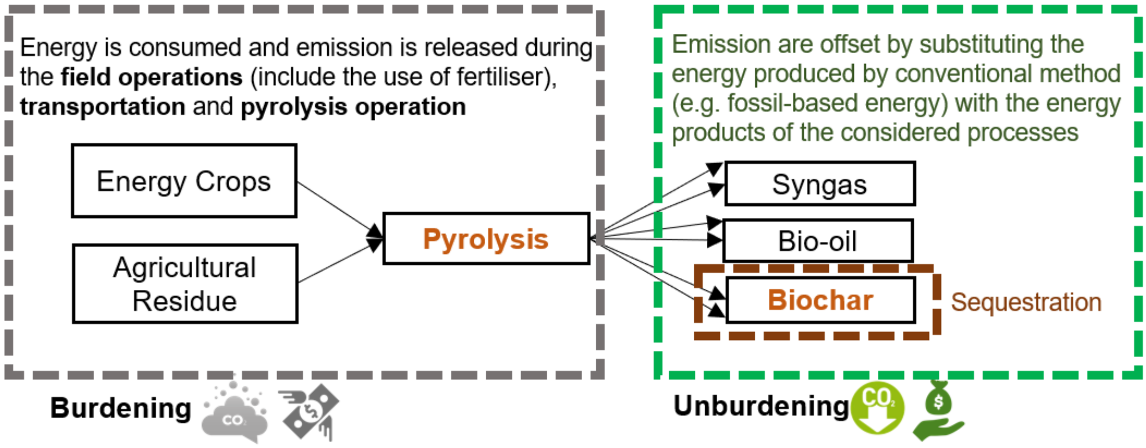


Figure 3.14: The overall assessment framework of the case study

Table 3.8: Scenarios description

Scenario	Description
1	Switchgrass (energy crop) + Pyrolysis optimised for energy (burn)
2	Switchgrass (energy crop) + Pyrolysis optimised for biochar (bury)
3	Wheat straw (agricultural residue) + Pyrolysis optimised for energy (burn)
4	Wheat straw (agricultural residue) + Pyrolysis optimised for biochar (bury)

Table 3.9: Data to construct a graphical decision-making tool. Extracted from Gaunt and Lehmann (2008)

	Unit	Scenario 1	Scenario 2	Scenario 3	Scenario 4
Amount of electricity	MWh ha^{-1} y^{-1}	17.98	13.67	11.22	8.52
Operating cost	USD ha^{-1} y^{-1}	205.90	205.90	27.81	27.81
Emission from operating process	kg ha^{-1} y^{-1}	6.62	11.41	8.20	14.20
Sequestrated emission	kg ha^{-1} y^{-1}	-	3,768	-	2,119

Price of electricity = 22.4 USD MWh^{-1} and Price of biochar = 0.047 USD kg^{-1}

3.2.4 Results and Discussion

Figure 3.15 shows the developed BBDM tool to compare (a) Scenario 1 and 2 as well as (b) Scenario 3 and 4. When there is no GHG charge (GHG price = 0), all the circumstances (energy crop or agricultural residue; small or large GHG intensity) suggest pyrolysis optimised for energy production. Burning the recovered products for energy provides a higher profit. The selection shift to pyrolysis optimised for biochar production with the increase of GHG price (> 0.03 USD/kg CO_2eq for switchgrass, >0.01 USD/kg CO_2eq for wheat straw), where the biochar is applied to the soil (bury). The GHG price is essential to encourage the application of biochar for GHG footprint reduction. However, burning is preferable with increasing GHG intensity. This is due to the higher footprints offset by displacing the dirty electricity grid mix (higher GHG intensity) with energy generated from pyrolysis. The applicability of the developed tool for decision-making can be demonstrated by using Country A (200 g CO_2eq/kWh) and Country B (1,000 g CO_2eq/kWh) as an example, at GHG price of 0.025 USD/kg (Plumper and Popovich, 2019). Figure 3.15a suggests the switchgrass in Country A and B is more suitable for energy production (burn) in order to have a higher total profit (earnings from selling the energy and the GHG credit). Figure 3.15b suggests the wheat straw in Country A should be utilised for biochar production but energy generation for Country B. To encourage the production of biochar (bury) in Country B, as illustrated in Figure 3.15b, the GHG price have to be increased, e.g. to 0.04 USD/kg.

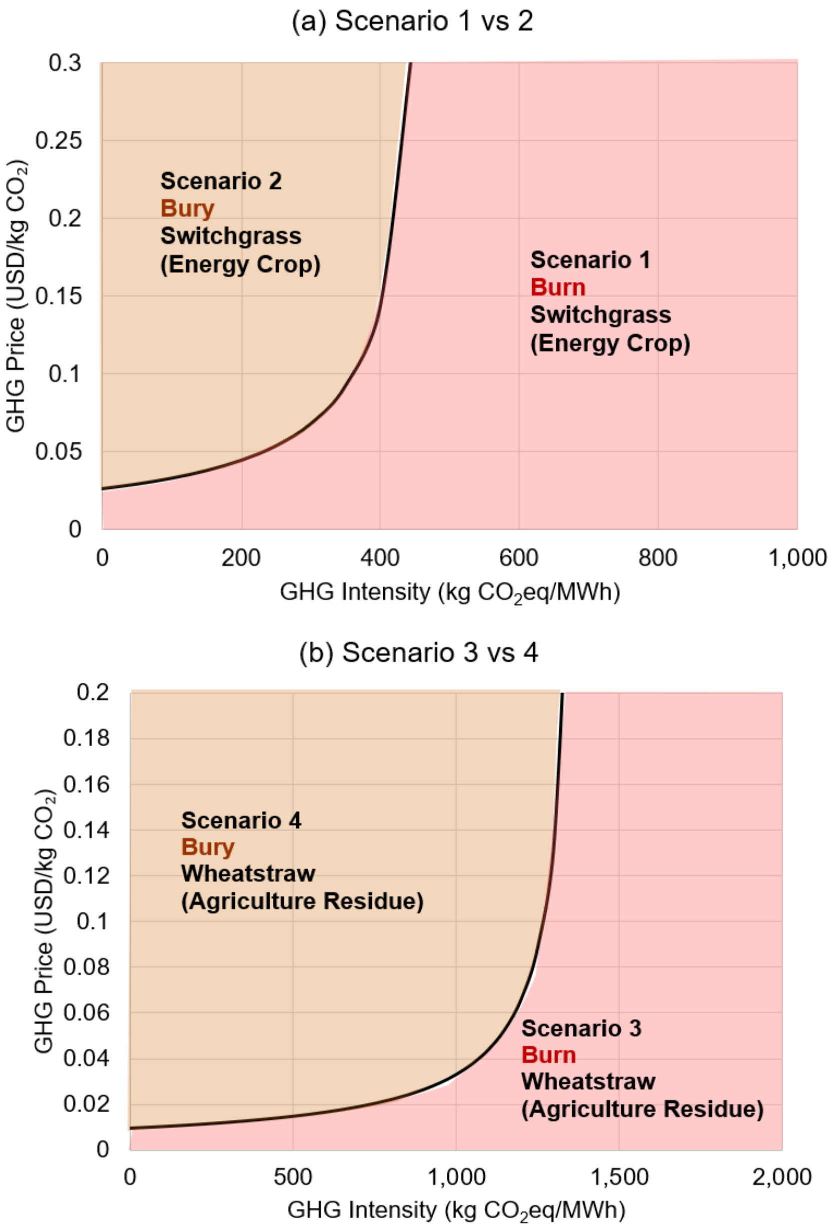


Figure 3.15: Graphical decision-making tool (burn or bury) for (a) Scenario 1 vs 2 and (b) Scenario 3 vs 4

Figure 3.16 shows the impact of substrate types to the break-even based decision-making tool. At 200 g CO_2eq/kWh (Country A), wheat straw is a better substrate for pyrolysis unless the GHG price is set to be higher than 0.02 USD/kg CO_2eq, see Figure 3.16a. Switchgrass, the dedicated biomass, has a higher net GHG footprint compared to wheat straw (agricultural residue) due to the burdening effect of field production in growing the switchgrass. However, switchgrass has a higher net GHG footprint with increasing GHG intensity, as reflected in Figure 3.16a (preferable options than wheat straw), due to the higher amount of energy from pyrolysis to displace the high GHG intensity energy mix.

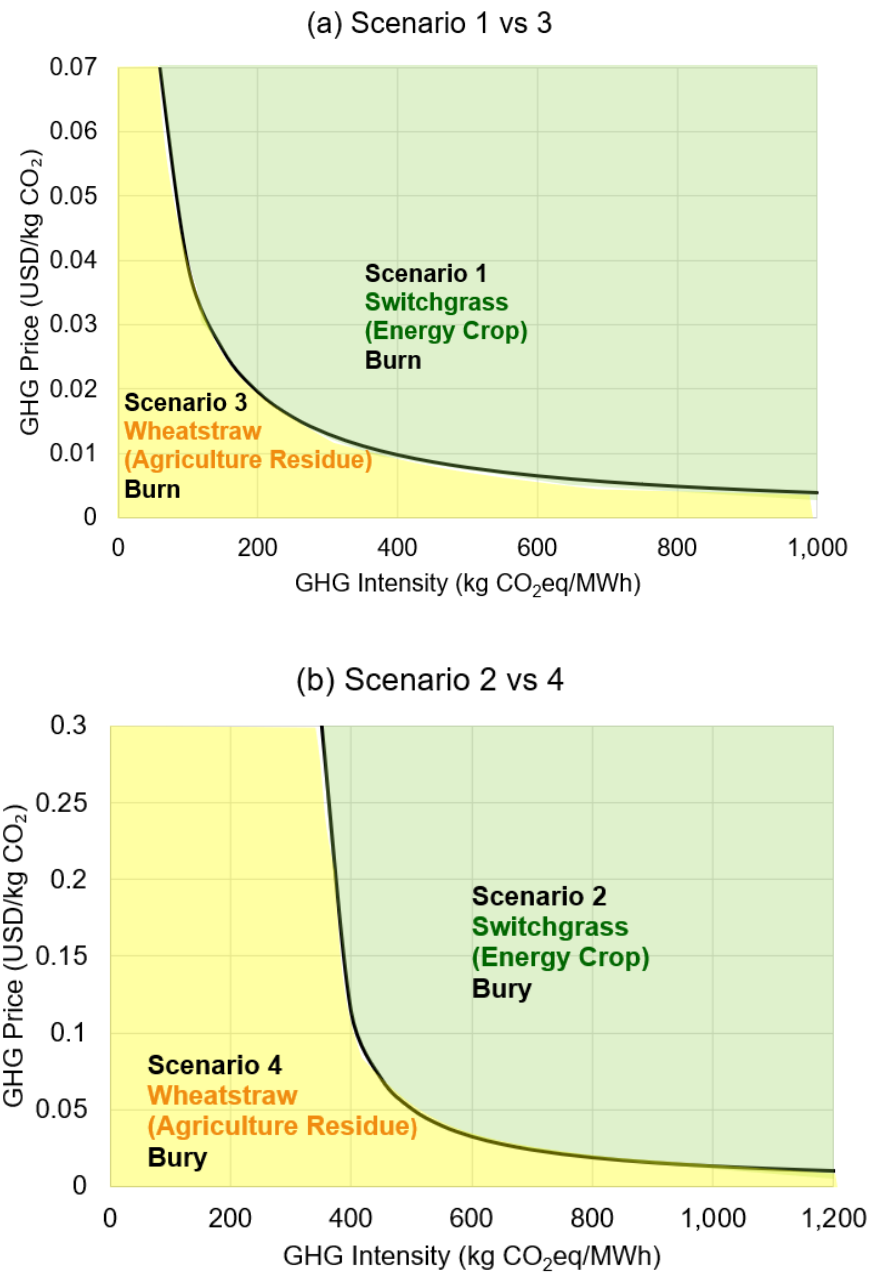


Figure 3.16: Graphical decision-making tool (types of substrate) for (a) Scenario 1 vs 3 and (b) Scenario 2 vs 4

3.2.5 Conclusion

The BBDM tool has been proposed as a means to determine the suitable biomass utilisation with highest possible profit and lowest GHG emission for a particular context with known GHG intensity and a defined GHG price. The tool provides rapid and effective decision support capability via an intuitive graphical display, in contrast to mathematical programming models. It is feasible for the comparison of different treatment options (e.g. gasification, pyrolysis and other waste to energy), technologies (pyrolysis in different setting e.g.

temperature), utilisation (energy, soil amendment, activated carbon), types of substrate and useful to capture the impacts contributed by the changes of GHG intensity and GHG price. The results of the pyrolysis case study show that burn is generally a preferable decision (at GHG price = 0) especially with the increase of GHG intensity, for both switchgrass and wheat straw. At GHG intensity = 200 g CO_2eq/kWh and GHG price = 0.025 USD/kg, pyrolysis of wheat straw is suggested to be optimised for biochar production and application to the soil (bury). However, at GHG intensity = 1,000 g CO_2eq/kWh, pyrolysis of wheat straw is suggested to be optimised for energy generation unless the GHG price is increased, e.g. to 0.04 USD/kg. Future studies should consider (i) a better accounting framework of biogenic and non-biogenic carbon as carbon neutrality cannot be assumed for all biomass energy a priori (ii) additional footprints (e.g. NO_x, SO_2, particulate matter) (iii) land availability and suitability for biochar application to improve the fidelity of the decision tools. The BBDM tool has a broader potential and flexibility for an extended application in decision-making. The presented case study shows one of the applications (biomass utilisation/treatment) however the similar concept/foundation can be applied to the different field; for example, transportation modes and fuel selection by using load and distance as the axes. The BBDM tool transforms the treatment/utilisation selection problem into an easily understandable format from which arises sound solutions.

CHAPTER 4

PINCH ANALYSIS TO MINIMISE THE EMISSIONS OF WASTE MANAGEMENT SYSTEM

4.1 Application to Municipal Solid Waste Management

The work presented in this section is based on the author publication in Chemical Engineering Transactions entitled "Extended Waste Management Pinch Analysis (E-WAMPA) Minimising Emission of Waste Management: EU 28", as clarified on Page V (Contributing publication). The author of this thesis is the first and corresponding author of this publication. The other co-authors who provided advices to this publication are the supervisor and Mr. Chin. My original contributions are listed in the introduction.

4.1.1 Introduction

Waste treatment plays an important part in the waste management system (WMS) after the effort of waste prevention. Improper waste management contributes to environmental issues such as greenhouse gas (GHG) emission, air, ground and water pollution. A wide range of waste recovery approaches includes material recycling, waste to energy and biological recovery have been introduced to support continuing economic growth and industrial development, by minimising the impact of waste generation. Recovery process consumes energy and releases GHG in the process of mitigating the footprints of waste. Various approaches have been applied to identify suitable waste treatment options and management systems. These include heuristic methods, multi-criteria decision analysis, graphs and network theory, mathematical optimisation, stochastic process techniques and statistical methods (de Souza Melaré et al., 2017). Ho et al. (2017) stated that most of the proposed model is performed by a "black box" mathematical optimisation approach, which is difficult to understand the reason in obtaining the optimal solutions fully. Studies proposed graphical approach is comparatively few. One such approach is the Pinch Analysis. This methodology has been widely applied to different fields and has the advantages to be easily understood. Linnhoff et al. (1982) are the foremost pioneers of Heat Recovery Pinch in solving the Heat Integration problem. There were various extensions of Pinch Analysis include for hydrogen integration, mass integration, water network synthesis, power system planning and regional resource planning (Klemeš et al., 2018). Tan and Foo (2007) developed an extension of Pinch Analysis as Carbon Emission Pinch Analysis (CEPA) for optimal allocation of energy sources based on the GHG emission constraints. It has been successful due to its capability to capture and communicate the challenge and opportunities in energy planning for low-GHG emissions. CEPA has been later introduced by Ho et al. (2017) to the waste management area as Waste Management Pinch Analysis (WAMPA). The modification includes (a) the non-carbon emitting option is 3R (reduce, reuse and recycling) instead of renewable energy as in the CEPA and (b) landfill reduction target is introduced. It was demonstrated by a hypothetical case study of five waste types. WAMPA approach has been later applied to a case study of China (Jia et al., 2018) using site-specific data. The y-axis and x-axis of WAMPA are GHG emissions and waste amount. The absolute value could mask some of the important information for an appropriate waste strategy planning, particularly if involving the net emissions accounting or comparison between countries. An improved method which considered the life cycle emissions (possibly using footprints) and a population of a country are needed. The country with high recovery rate is not necessary the countries with the lowest emission as the waste amount could be significant.

The presented study introduces the intensity of WMS as the selecting approach in identifying the potential of a country for improvement (emission reduction). It represents net emission per capita (in this study specifically to GHG). The net GHG emission is accounted by the amount of emission emitted from the treatment processes and the emission mitigated from material reprocessing and avoided primary production. The study aims to propose a graphical approach in identifying the WMS (a set of waste treatments) with lower emissions. The proposed graphical approach is an extension to the existing WAMPA, which is extended initially from CEPA approach, inspired by the concept of Pinch Analysis. In this study, the approach is referred to as E-WAMPA, representing Extended-WAMPA. The applicability of E-WAMPA is demonstrated through a case study of the EU. It facilitates the waste treatment selection by suggesting the strategies (share of different waste treatments) based on defined targets (e.g. recycling rate, waste amount, landfill reduction). **My novel contributions include:**

(i) The intensity of the WMS (Net GHG emission per capita) is introduced as an indicator of the potential reduction of a country. It could better reflect the net emission of a country than the absolute value.

(ii) The step by step algorithm of WAMPA is improved by considering the limitation in developing WAMPA. For example, the assumptions of 3R activities have no emission, WtE is given priority over 3R due to energy production and economic reasons, which are not truly reflecting the real-life condition.

(iii) The applicability is demonstrated by EU-28 case study rather than a hypothetical case study. The demonstration is based on the defined targets and projection of the EU. E-WAMPA is capable in proposing a WMS that meeting the emission reduction targets of a country, region or globally.

4.1.2 Method

The methodology is divided into two major sections. Section 4.1.2.1 and 4.1.2.2 present the generic method that independent of the case study. The approach in identifying the emission intensity of waste treatment practices in a place is presented in Section 4.1.2.1. A step by step algorithm of E-WAMPA in identifying the potential mitigation strategies is introduced in Section 4.1.2.2.

4.1.2.1 Emission Intensity of Waste Management System (WMS)

The emission intensity of the WMS is determined by using Eq(4.1). Emission intensity including carbon emissions intensity has been commonly used as an indicator to evaluate the environmental performance of energy source in the unit of CO_2eq/GDP (Dong et al., 2018), where a lower value is representing a greener energy source (e.g. higher share in renewable energy). Eq(4.1) is based on a similar idea, but the emissions are divided by population. It is determined by summing the net emission contribution of each waste treatment alternatives ($E_{\mathrm{emitted}} - E_{\mathrm{avoided}}$, t of emissions) divided by population (p, capita). This study considers GHG (CO_2, CH_4, N_2O), but further emissions can be accounted for by this approach as well.

$$T_{\mathrm{netEwaste/cap}} = \frac{\sum_t (E_{\mathrm{emitted}} - E_{\mathrm{avoided}})}{p} \tag{4.1}$$

Where t is representing the waste treatment alternatives, E_{emitted} is the emission release by the waste treatment processes, E_{avoided} is the emission mitigated by primary production and material reprocessing (Fan et al., 2019c). For example, the emission mitigated by the energy produced from incineration. The mitigated emission is based on the current practice of energy production, and different countries have a different magnitude of saving due to the different energy mix. The lower value of WMS emission intensity ($T_{\mathrm{netEwaste/cap}}$) represents the environmental performance better. In some cases, the value is in negative and suggests the waste treatment practices achieve emission saving (Turner et al., 2015). It may be through recycling as it can replace the primary production of virgin products. It does not represent the achievement of sequestration as the assessment boundary does not include the emission of waste production.

4.1.2.2 Pinch Analysis

This section presents the E-WAMPA framework for extended application in waste management. The definition of Pinch Point and the Demand Curve are the same as of WAMPA (Ho et al., 2017), refer to the emission reduction target. Waste treatment alternatives and countries represent the Supply Curve. E-WAMPA is presented as a 2D-graph where the x-axis is the cumulative waste amount, and the y-axis is the cumulative emissions (NetGHG emission). The generic step by step algorithm of E-WAMPA:

(i) Step 1, Supply Curve 1 (the red line):
Construct the stacked curve of countries (Figure 26) using the cumulative waste amount as the x-axis and cumulative emission (NetGHG emission) as the y-axis. The countries are arranged in a sequence based on emission intensity (Net GHG emission per capita). The countries arranged at the end of the cumulative curve represent the countries where the environmental performance of the WMS has an increasingly larger room for improvement. It will be the targeted countries to be altered for meeting the reduction target.

(ii) Step 2, Supply Curve 2 (the red line):
Construct the stacked curve based on the treatment system of targeted countries as in Step 1. In this study, the Supply Curve 2 represents by the Recycling Curve, Energy Recovery Curve, Composting and Anaerobic Digestion Curve, Disposal by Incineration Curve and Landfill Curve, following the classification by the EU. The treatment alternatives are arranged by sequencing based on the increasing net emission per amount of waste processed. The net emission per amount of waste processed varies across the countries mainly as the energy mix is different, contributing to the different E_{avoided}.

(iii) Step 3, Optional (the yellow line):
In this specific case study (see Section 4.1.3), an additional line/curve is constructed. It represents the waste treatment situation of the EU country in the year of 2017. It is mainly to show the changes in the waste amount in 2030. This provides a picture closer to the real-life situation as the waste amount change (either increase or decrease) along at the defined future target of emission reduction and WMS.

(iv) Step 4, Target:

The emission reduction target of a region is defined. E.g. In the case study, the reduction target of EU-28 is to minimise overall emission by 10 %. That is the target (Pinch Point) to be achieved.

(v) Step 5, Pinch Analysis - The Shifting (labelled as the green line):

Shift the Supply Curve 2 based on the define targets of waste treatment options. Adjust the amount of waste to the other recovery or disposal options until the target at Supply Curve 1 is satisfied.

4.1.3 Case Study

The proposed methodology is demonstrated using the EU-28 scenario. The considered countries include Austria (AT), Belgium (BE), Bulgaria (BG), Croatia (HR), Cyprus (CY), the Czech Republic (CZ), Denmark (DK), Estonia (EE), Finland (FI), France (FR), Germany (DE), Greece (EL), Hungary (HU), Italy (IT), Latvia (LV), Lithuania (LT), Luxembourg (LU), Malta (MT), Netherlands (NL), Poland (PL), Portugal (PT), Romania (RO), Slovakia (SK), Slovenia (SL), Spain (ES), Sweden (SE) and the United Kingdom (UK). Ireland has not been included as the data were not found. Table 4.1 shows the input data required to estimate the E_{avoided} and E_{emitted}, see Eq(4.1).

Table 4.1: The emission/output of waste treatment and disposal processes

Treatment	Emission	Output	Comment
Landfill	568 kg CO_2eq/t[e]	-	-
Incineration	386 kg CO_2eq/t[c]	315 kWh/t[a], 795 kWh/t[b]	For disposal, energy is not recovered.
Composting	26.3 kg CO_2eq/t[d]	600 kg/t of compost[j]	Compost contains 0.03 % of nitrogen. 3.6 t CO_2eq/t N[h]
Anaerobic digestion	228.5 kg CO_2eq/t[f]	150 m^3/t of biogas, 1.81 kWh/ m^3 [a], 2.27 kWh/ m^3 [b], 0.9t/t of digestate[i]	Digestate contains 0.01 % of nitrogen. 3.6 t CO_2eq/t N[h]
Recycling	Net GHG= - 845.35 kg CO_2eq/t[g]		MSW consists of 55 % paper, 21 % plastic, 9 % glass, 15 % metal

[a]electricity, [b]heat, [a,b,c,d](Thinkstep AG, 2017), [e](Ritchie and Smith, 2009), [f](Phong, 2012), [g](Turner et al., 2015), [h,i](Fan et al., 2018b), [j](Fan et al., 2018c)

Table 4.2: Data inputs of EU case study

	Waste amount (kt)		Population (M cap)		CO_2 intensity[c] (gCO_2/kWh)	Share (%), 2017[d]				
Country	2017[a]	2030[b]	2017[a]	2030[b]		Landfill	D10	R1	R	C&A
AT	5,018	5,352	8.803	8.946	85.1	2	0	39	26	32
BE	4,659	5,350	11.391	12.002	169.6	1	1	43	35	20
BG	3,080	3,306	7.080	6.431	470.2	62	0	3	27	8
HR	1,716	1,703	4.125	3.896	210.0	75	0	0	22	2
CY	547	624	0.858	1.282	676.9	82	0	0	15	2
CZ	3,643	3,848	10.590	10.528	512.7	48	0	17	27	7
DK	4,503	4,983	5.765	6.025	166.1	1	0	53	27	19
EE	514	523	1.317	1.254	818.9	21	0	47	28	4
FI	2,812	3,080	5.513	5.739	112.8	1	0	59	27	13
FR	34,393	36,021	67.042	67.894	58.5	22	0	35	24	19
DE	52,342	54,400	82.688	82.187	440.8	1	4	27	49	18
EL	5,415	5,966	10.744	10.784	623.0	80	0	1	15	4
HU	3,768	3,886	9.787	9.235	260.4	49	0	16	27	8
IT	29,583	29,855	60.496	58.110	256.2	26	1	20	31	22
LV	851	882	1.942	1.747	104.9	51	0	5	31	13
LT	1,286	1,382	2.826	2.718	18.0	33	0	18	24	24
LU	362	434	0.596	0.675	219.3	2	0	15	10	73
MT	283	304	0.468	0.440	648.0	93	0	0	7	0
NL	8,787	9,816	17.128	17.594	505.2	1	1	43	26	28
PL	11,969	12,001	37.996	36.616	773.3	42	2	23	27	7
PT	5,012	4,890	10.291	9.877	324.7	50	0	21	12	18
RO	5,325	5,301	19.577	18.464	306.0	80	0	5	8	7
SK	2,058	2,024	5.444	5.387	132.2	61	0	10	21	9
SL	974	1,030	2.067	2.059	254.1	13	0	10	56	21
ES	21,530	21,226	46.601	46.115	265.4	54	0	13	18	15
SE	4,551	5,123	10.068	10.712	13.3	0	0	53	31	15
UK	30,911	36,720	66.049	70.579	281.1	17	1	37	28	17

[a,d](Eurostat, 2019), [b](Kaza et al., 2018), [c](EEA, 2018). D10 = incineration (disposal, without energy recovery), R1 = energy recovery, R = material recycling. C & A = composting and anaerobic digestion. The 2030 projection is based on the year of 2015 by Kaza et al. (2018). Some of the data might not be able to reflect the exact situation, but it is based on the collected data from the sources as cited. The accuracy of the data is not the main issue as it is mainly used to demonstrate the applicability of the proposed method.

Table 4.2 shows the data inputs of the EU. The carbon emissions intensity is used to identify the emission saving from energy recovery processes. The increase in the waste amount in the year 2030 is assumed to be handled based on the same practices (% of share) as in 2017. The common EU target has been 65 % recycling of MSW by 2030 and reduces landfill to a maximum of 10 % (EC, 2017). The situation in EU countries is varying where some of the countries have already achieved the 10 % landfill target. The priorities of shifting are targeted for the countries with high net GHG emission per capita as described in Section 4.1.2.2, Step 1. The target/pinch point of this case study is to reduce the net GHG emission of EU WMS by 10 %, and the waste to the landfill has to be reduced by 50 %.

4.1.4 Results and Discussion

Figure 4.1 shows the cumulative emission and waste amount of the assessed EU countries in 2017 (yellow line) and 2030 (red line), arranged in increasing emission intensity. The average emission intensity of the EU is -0.05 tCO_2eq/cap. Germany, Slovenia, Netherlands, Estonia, Denmark and Belgium are well above the average. Germany is one of the top ten countries with the high absolute amount of waste (Table 4.2), but in tCO_2eq/cap it has the best performance, contributed by the WMS which capable in mitigating the footprint of waste and lower waste generation per capita. Malta, Greece, Cyprus and Romania, which located at the end of the red line are the selected countries for improvement. The demonstrated case study focuses on only one strategy- treatment transition (switch to treatment options with lower emission). The other possible strategies are waste trading (import and export activities based on treatment capacity) and enhancing treatment efficiency.

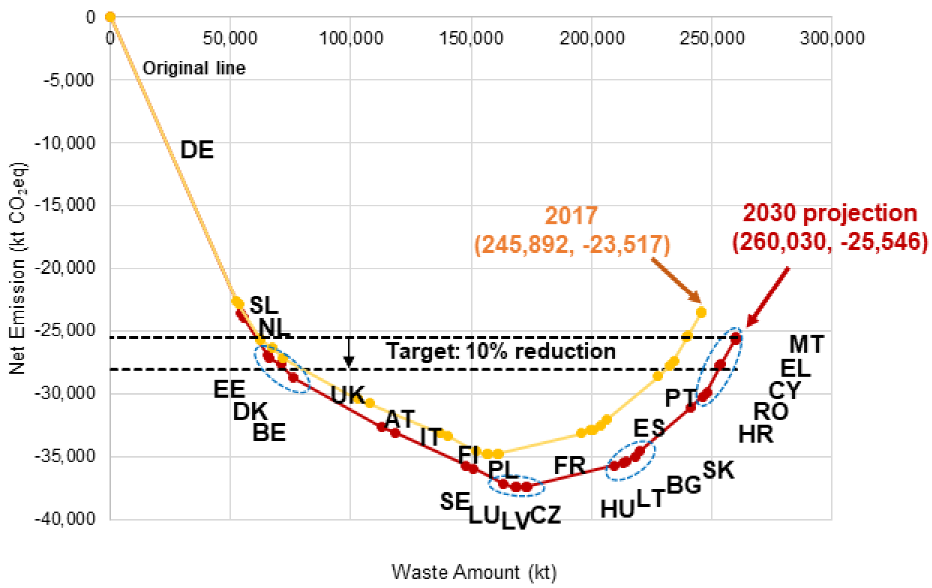


Figure 4.1: E-WAMPA for the waste management system of EU counties in 2017 and 2030 - Supply Curve

Figure 4.2 shows the shifts (treatment transition) in Malta, Greece, Cyprus and Romania contribute to the reduction of EU emission of WMS (-25,546 to -28,114). Following the E-WAMPA methodology, one of the possible solutions is:

i. In Malta (MT): send 50 % waste for landfill to D10
ii. In Greece (EL): send 50 % waste for the landfill to D10, R1, C&A
iii. In Cyprus (CY): send 50 % waste for the landfill to C&A
iv. In Romania (RO): send 50 % waste for the landfill to R1 and D10

The shifting contributed to the decrease (10%) in the overall WMS emission of EU and met the Pinch point (Figure 4.3). The zoomed view shows the shift where waste emissions are reduced despite handling the same amount of waste (260,030 kt). Data availability on the waste treatment capacity could further improve the feasibility of the allocation and waste trading.

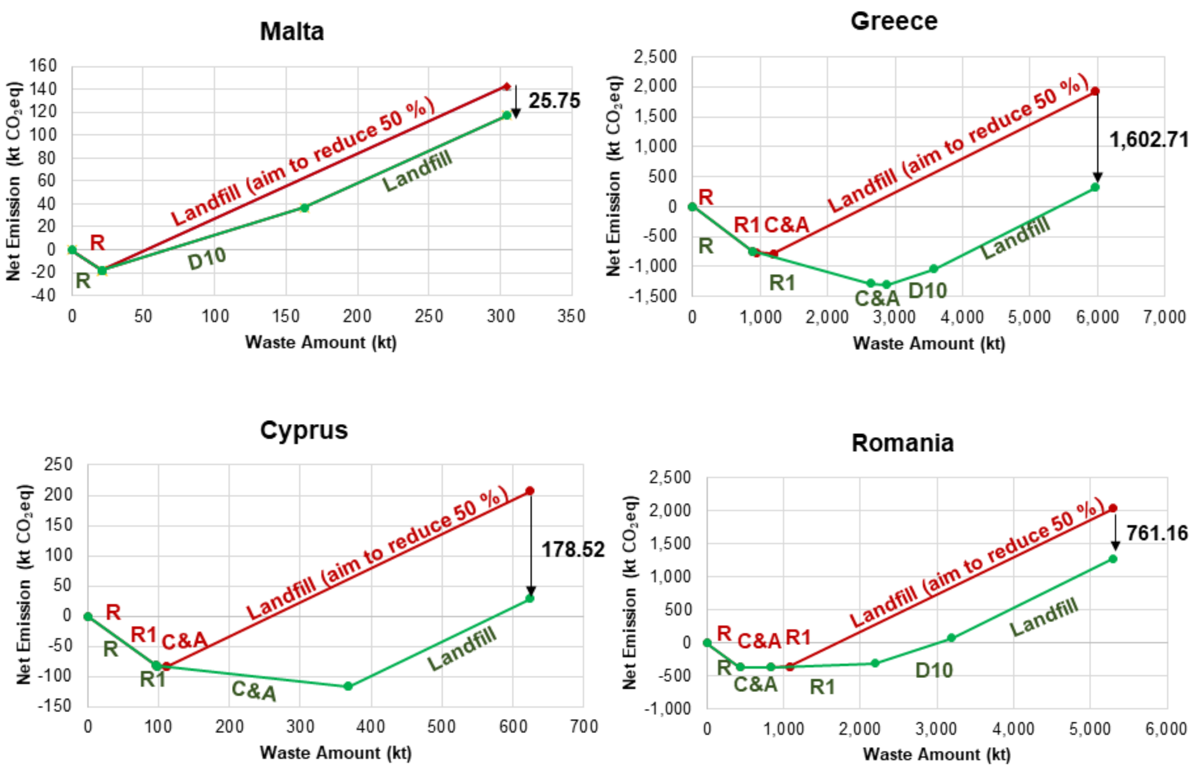


Figure 4.2: Treatment transition of Malta, Greece, Cyprus and Romania

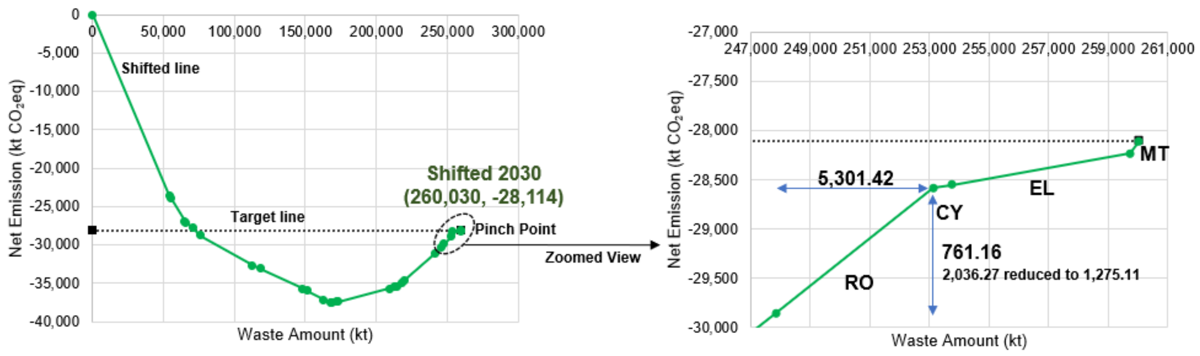


Figure 4.3: E-WAMPA for the waste management system of EU countries- Shifted Curve and its zoomed view

Economic feasibility of a waste management system has always been a significant challenge. It was reported that the operating cost including collection, transport, treatment and disposal in a high-income country generally exceed \$100/ t (Kaza et al., 2018). Lower-income countries spend less on waste operation at the cost of about \$35/t (Kaza et al., 2018). However, the cost should not be limited to the direct profit or benefit rather than a broader perspective. The environmental and social impacts reduction is indirect profit, and they are the essential driving force in realising the treatment transition. Treatment transition has been more recognisable with the introduction of the circular economy concept, carbon taxes, and changes of government policies. According to the circular economy concept, waste is view as secondary resources. The resources are at low cost and can be recycled or recovered as new products, potentially reduce environmental footprints. In line with the EU priority to circular economy policies (EuroStat, 2018), the proposed methodology (E-WAMPA) is designed as a potential methodology to facilitate decision making. It is targeted on the EU countries, which have a higher potential for emission reduction, and the common/ individual targets can be predefined. Future work can integrate the circular indicator of EU to the proposed methodology and refer to the EU ambitious in treatment transition. For example, recycling 70 % of specific packaging materials (EC, 2017). The methodology is designed in a way that the common EU emission reduction can be achieved by improving the treatment transition of any of the EU members based on the potential. The potential can be referred to as treatment capacity, financial, waste handling technologies, the demand for recovered product or utilities. All these potentials will be further studied and incorporated into E-WAMPA for a more comprehensive algorithm.

4.1.5 Potential Extension and Strategy for Further Emission Reduction

The results presented in Section 4.1.4 are focused on waste treatment transition. Waste trading is an alternative strategy which could potentially further reducing the emissions. It could be a more promising strategy than treatment transition in the sense that current system design is in the transition towards a circular economy or zero waste target. Building new facilities or infrastructure to manage the waste is in contradiction to the waste prevention action plan. The cost of building a new treatment plant and social acceptance is also the challenges of waste treatment transition. Waste trading (import and export activities based on available treatment capacity) on the other hand, offers the sharing of resources and facilities to achieve a mutually beneficial design. The similar framework as presented in Section 4.2 (Application to Biomass Management) can be applied to facilitate this integrated regional planning (waste trading).

Figure 29 illustrates the framework for integrated regional waste management planning (waste trading). The presented values in Figure 29 are hypothetical with the intention to demonstrate the potential extension. The graphical targeting tool by Ooi et al. (2013) based on Pinch Analysis can be modified and integrated with BBDM to address the waste trading planning problem. The x-axis and Composite Curves have to be adapted to the waste management cases as the proposed targeting tool is originally for carbon capture and storage planning. Figure 4.4a shows an example of the Composite Curves where the capacity of the treatment plants are higher than the source (waste to be treated), with a surplus, at all the time interval. Figure 4.4b shows an example of the Composite Curves where at some of the time interval, source to be treated is higher than the capacity. At 8 and 10 weeks, there is a capacity surplus. The treatment capacity at that time interval cannot be brought forward. However, the source can be stored and treated when there is available treatment capacity or send to other countries for treatment.

Figure 4.4c shows an illustrative example of combined or merged available source and capacity of different countries after optimising locally (e.g. within a country). The countries (e.g. EU) can complement each other by sharing the treatment facilities which have not been fully utilised through an integrated system. The waste management planning should be able to response accordingly to the changing waste amount (fluctuating) and the available treatment capacity in each time interval. To match the available capacity, the blue source composite curve in Figure 4.4c can shift to the right until it touches the orange capacity composite curve at 10 weeks (see Figure 4.4d). The gap at 0 week shows the additional waste amount that can be handled.

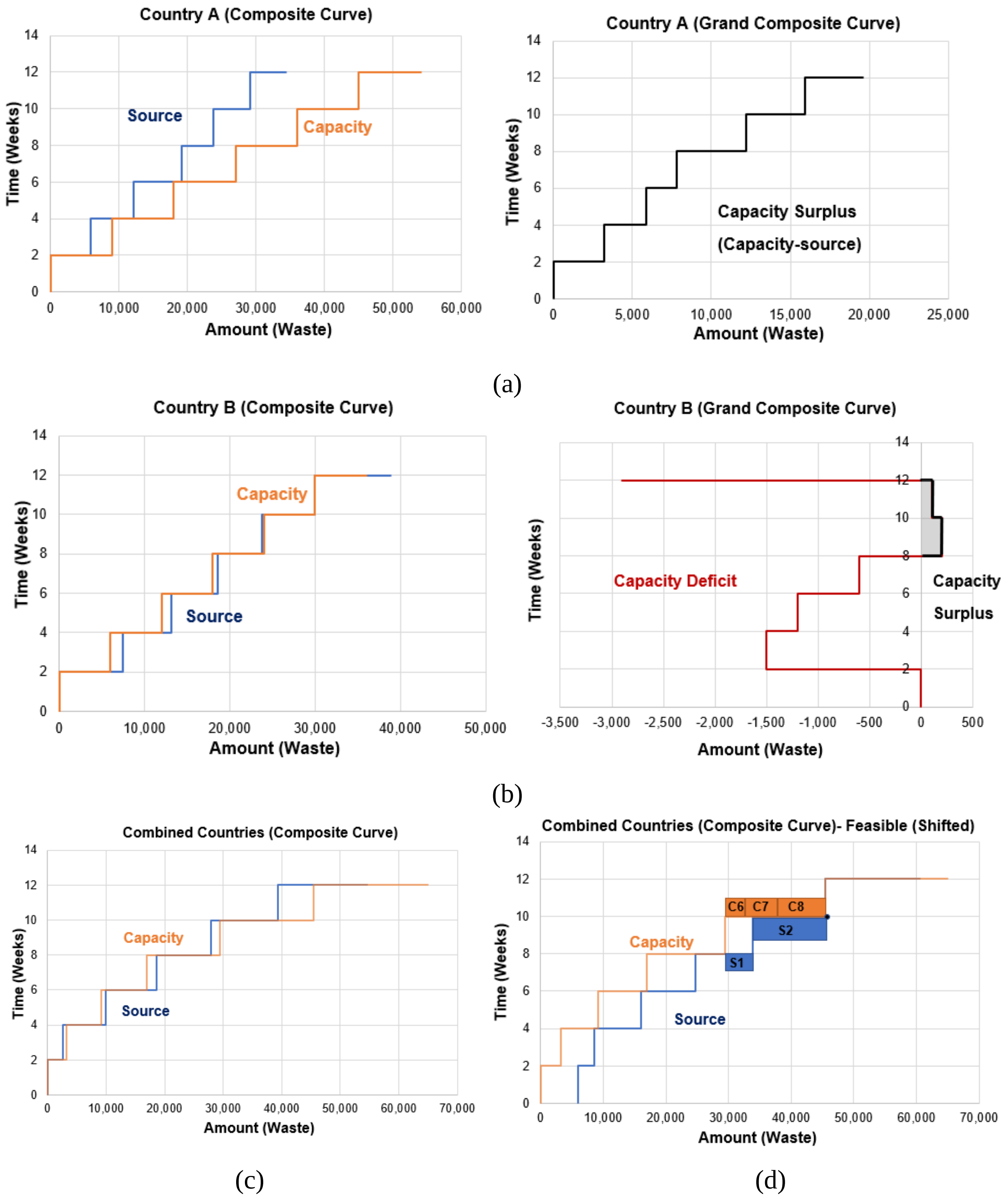


Figure 4.4: Proposed framework - Extension of Pinch Analysis for integrated regional waste management planning by waste trading (a) Composite Curve and Grand Composite Curve of Country A – example with surplus (b) Composite Curve and Grand Composite Curve of Country A – example with surplus and deficit (c) Example of Combined Composite Curves. (d) Example of shifted Combined Composite Curves. S = source, C = capacity.

The fundamental concept of this allocation and scheduling approaches have been proposed by Ooi et al. (2013) for carbon capture and storage planning. However, the main consideration is focused on matching the availability (supply and demand). The emissions, for example, from allocating activities have not been included. By referring to Figure 4.4d (at 8 and 10 weeks), the total waste amount and treatment capacity are the combined value of S1, S2 as well as C6, C7 and C8. The optimal allocation (which source to which capacity) can be determined by assessing the costing or the emission footprint. The optimal selection can be based on BBDM as in Chapter 3 or mathematical optimisation as in Section 4.2. Contour plot (as in Figure 4.5) with the load, distance and emission as axes can also facilitate the decision making. For example, by comparing the emissions by different transport mode (e.g. container ship and train) from location S1 to C6, C7, C8 versus S2 to C6, C7, C8, where the pairing with lowest emissions will be the allocation of waste trading.

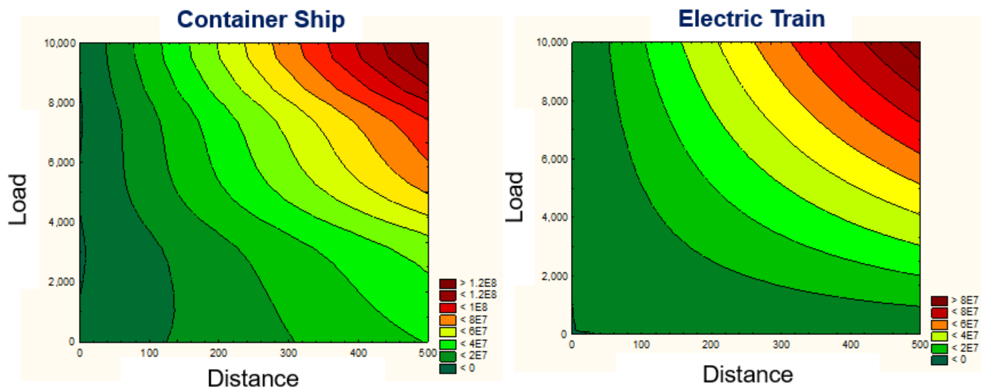


Figure 4.5: Examples of graphical representation to facilitate decision making (a) container ship (b) electric train. The colour scale represents the range of emissions (amount)

The Pinch Analysis based framework integrated with Breakeven based decision making or mathematical optimisation is a potential extension for further emission reduction. It could be effective in facilitating the waste trading planning (inventory, maximising capacities and sourcing) by well-managed complementation among regions or countries through resources sharing. However, a thorough assessment is required for establishing the regulation and incentive of the trading system.

4.1.6 Conclusion

This work proposed E-WAMPA to facilitate the waste allocation in WMS towards emission mitigation graphically. The applicability of E-WAMPA is demonstrated through a possible reduction strategy (treatment transition). Malta, Greece and Cyprus and Romania are chosen as the demonstrated countries as the net GHG emission from the waste treatments per capita are high, representing the room for improvement toward emissions reduction of EU. The future research will further elaborate on the E-WAMPA methodology. The extended potential for proposing a WMS by considering the variation in waste amount and composition while meeting the treatment target and the overall emission reduction target of a region will be demonstrated. The additional future scope includes integrating the waste transportation issues (supply chain), virtual footprints, energy return on investment of waste treatment process as well as a circular economy concept to E-WAMPA.

4.2 Application to Biomass Management

The work presented in this section is based on the author publication in Chemical Engineering Transactions entitled "Biomass Supply and Inventory Management for Energy Conversion", as clarified on Page V (Contributing publication). The author of this thesis is the first and corresponding author of this publication. The co-author is the supervisor (Prof Klemeš). My original contributions are listed in the introduction.

4.2.1 Introduction

Biomass to energy conversion receives increasing attention due to the concerns on energy security and GHG emissions from fossil fuel consumption. The sources of biomass are the forest, edible crops, dedicated biomass, residues and waste. The main challenge of the biomass supply chain is the source which is disseminated over a large area and influenced by a strong seasonality (Lautala et al., 2015). Acuna et al. (2019) divide the biomass supply chain decisions into strategic, tactical and operational levels. The efficiency of supply chain management is crucial for the economic and environmental viability of the conversion plant. Mathematics optimisation has been essential in facilitating the decision making of this complex management. The other methods are a simulation, geographic information system, and heuristics. Mixed-integer linear programming and multi-criteria decision analysis among the most applied method. How et al. (2016) integrates P-graph framework and mathematical modelling to identify the optimal number and location of hubs as well as the allocation design. Akgul et al. (2014) applied Mixed-integer nonlinear programming to determine the optimal design of a bioelectricity supply chain in the UK by optimising the cost and emission. Shabani et al. (2016) consider the uncertainties in biomass quality by stochastic programming. Lim et al. (2019) tackle the insecure supply of biomass by using element targeting approach and multiperiod analysis. Zandi et al. (2018) highlighted that the studies integrate decisions such as plant localisation and dimensioning in biomass supply design is scarce.

Pinch Analysis (Linnhoff et al., 1982) is one of the potential methods. It is originally for heat integration problem and has been extended widely in recent years (Klemeš et al., 2018). This targeting approach with graphical representation is suitable for practical purpose, easier to understand by the practitioner and serve as an excellent platform in minimising the problem size for the following detail planning. Lam et al. (2011) apply the Pinch concept and clustering approach for regional resource management. Production Pinch Analysis is among the graphical heuristic method, which could be used for biomass supply chain planning. It has been proposed by Singhvi and Shenoy (2002) in general for supply chain planning, to identify the production rate for a given demand forecast. A total of 6 Pinch production strategies have been later summarised by Ludwig et al. (2009). However, the proposed approach has not been well demonstrated through biomass supply chains case study. The main discussion is focused on interpreting the possible strategies. This study aims to integrate Pinch Analysis for targeting and mathematical model for the follow-up optimisation of the production rate, product inventory (e.g. bio-oil), biomass storage and biomass network flow (allocation). **My novel contributions include:**

(i) Embedding Process Integration into biomass utilisation planning to overcome the fluctuating supply and demand of energy conversion

(ii) Integration of extended production Pinch Analysis and mathematical optimisation in satisfying the energy demand under the fluctuating biomass supply to maximise the profit through inventory minimisation.

(iii) Optimised the biomass allocation by reducing the cost incurred in transporting and carbon tax

4.2.2 Method

4.2.2.1 Pinch Analysis

Pinch Analysis for aggregated planning by Singhvi and Shenoy (2002) is adapted to estimate the possible production rate and inventory level of biomass to energy conversion. Y-axis is replaced with energy to fit the purpose of the case study. The profit is maximised by minimising the inventory (product accumulation). Insufficient inventory to fulfil the demand leads to a loss in sales and profits while a surplus of inventory results in unnecessary costs. Figure 4.6a shows the composite curves example and its interpretation. The Composite Curves are Demand Curve and Production Curve. Demand Curve is plotted by cumulative demand at different time. Production Curve is identified by rotating the horizontal axis from the starting inventory as the pivot until it touches the Demand Curve as described by Singhvi and Shenoy (2002). Grand Composite Curve is plotted by minus the Production Curve by Demand Curve. It is a graphical representation that useful in showing the distribution of product inventory (e.g. bio-oil accumulates) at various time. The supply of biomass is subjected to seasonality and availability. Biomass storage is needed to fulfil the demand and production rate at each time interval. It can be determined by further extending the Pinch Analysis (see Figure 4.6b), where a grand composite curve is plotted by minus Supply Availability Curve by Production Curve for excessive availability of supply. The required supply (and hence the biomass storage for low supply period) at a various time can be identified for further biomass flow (from which source and its amount) optimisation.

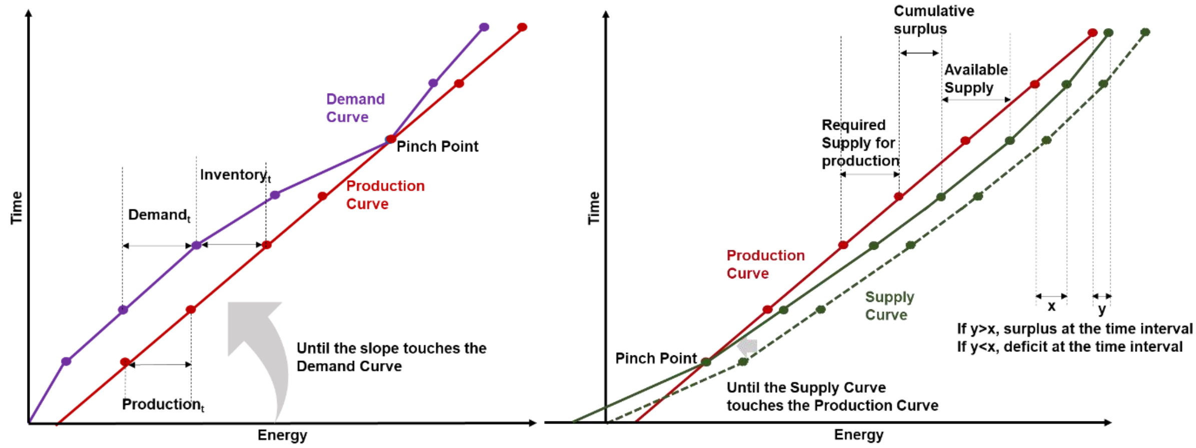


Figure 4.6: Composite Curves of aggregate planning in supply chain (a) Demand (Purple) and Production (Red) Curve; (b) Production (Red) and Supply (Green) Curve

4.2.2.2 Optimisation model

The biomass flow (sources - location and amount) is identified by Eq(4.2) and Eq(4.3) with the consideration of energy content (GJ/ t) of biomass, transporting distance, load (required supply) and the number of the trip. The identified required supply at a various time by Pinch Analysis has to be fulfilled. The objective function is minimising the cost, includes both transportation and GHG emission.

$$Min_{cost} = \sum_{k} (n \cdot e_{empty} + L \cdot e_{load}) D_k \times GHG_{cost} + (L_k \times D_k \times T_{cost}) \tag{4.2}$$

$$n = Roundup\left(\frac{L}{W_{max}}\right)\ and\ n \in Z^{+} \tag{4.3}$$

Where e_{empty} is the specific emission of an empty transport vehicle fleet (g/km); e_{load} is the marginal specific emission of a transport vehicle fleet per t of transport load (g/tkm); n is the required number of transport vehicles; D is the transport distance that each vehicle has to travel (km), and L is the total transport load across all vehicles (t). GHG_{cost} is the GHG pricing (e.g. carbon tax), T_{cost} is the transporting cost; k is the source of biomass, in this study labelled as S1-S6. $W_{max}$is the maximum capacity of the transport mode. Eq(4.2) is accompanied by two constraints listed in Eq(4..4) and Eq(4.5). The total supply amount ($S_{k)}$) multiply by energy content per t of biomass (EC_k) and energy conversion efficiency (CE) has to equal to the identified necessary supply (IRS) at each time intervals. The amount of supply at each source point (S_k) cannot exceed its available supply.

$$IRS = \sum_{k}(S_k \times EC_k \times CE) \tag{4.4}$$

$$S_k \leq Available\ supply \tag{4.5}$$

4.2.3 Case Study

The method is demonstrated through a case study where 6 locations with different type and amount of biomass are illustrated, as in Table 4.3 and Figure 4.7. The energy demand (bio-oil) in 6 different months is listed in Table 4.4. Table 4.5 shows the other information for targeting and optimisation. The energy conversion of this study is assumed as 60 %, and the transporting mode is lorry with the specification as in Table 4.5.

Table 4.3: Source of biomass

Source Location	Energy Content (GJ/t)	Available Biomass Supply (t)					
		Month 1	Month 2	Month 3	Month 4	Month 5	Month 6
S1	17.17	0	300	0	0	300	0
S2	18.58	2,000	1,800	0	0	100	0
S3	19.3	100	0	0	0	300	0
S4	14.83	0	300	0	100	0	100
S5	20.81	0	0	700	500	0	0
S6	20.81	300	0	800	500	0	0

Table 4.4: Energy demand at each time interval

Month	Energy Demand (GJ)
1	20,000
2	7,000
3	40,000
4	3,000
5	5,000
6	10,000

Table 4.5: Input data

Other Information	Assumptions/ Value	Reference
Pyrolysis	60 % conversion efficiency	
GHG Price	56.6 €/t	CE Delft (2017)
Transporting Cost	0.16 €/tkm	IEA (2019)
Transportation	Emission factor = 76 g/tkm	Boer et al. (2016)
mode (Lorry)	Weight of empty lorry (Bodyweight) = 60 t	Boer et al. (2016)
	Maximum capacity = 40.8 t	Boer et al. (2016)
	e_{empty} = 1,845.71 g/km; e_{load} = 30.76 g/tkm	Fan et al. (2019a)

The location of treatment plant (pyrolysis) is proposed by using the centre of gravity method, as reviewed by Onnela (2015), considering the distance and biomass availability, see Eq(4.6) and Eq(4.7). The Euclidean distance, which is rotational invariance, can be identified by Eq(4.8). The route distance can be applied if the data is available (e.g. by Geographic Information System) The biomass flow (in each location and months) is optimised using Eq(4.2) after targeting by Pinch Analysis.

$$x_t = \sum_k x_k . A_k \div \sum_k A_k \tag{4.6}$$

$$y_t = \sum_k y_k . A_k \div \sum_k A_k \tag{4.7}$$

$$D = \sqrt{(x_k - x_t)^2 + (y_k - y_t)^2} \tag{4.8}$$

x_t is the x coordinate of the optimal treatment plant location; y_t is the y coordinate of the optimal treatment plant location; x_k is the x coordinate of the biomass source, y_k is the y coordinate of the biomass source; A_k is the available supply.

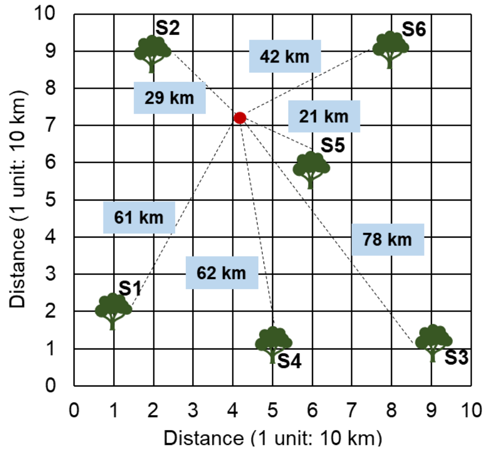
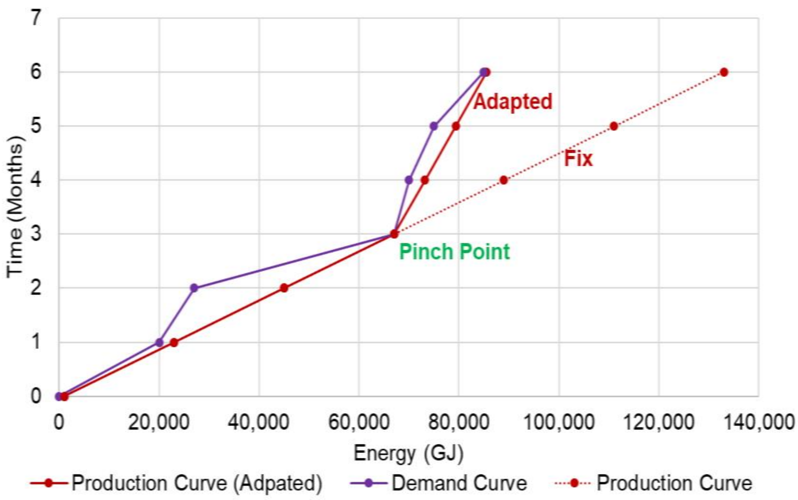


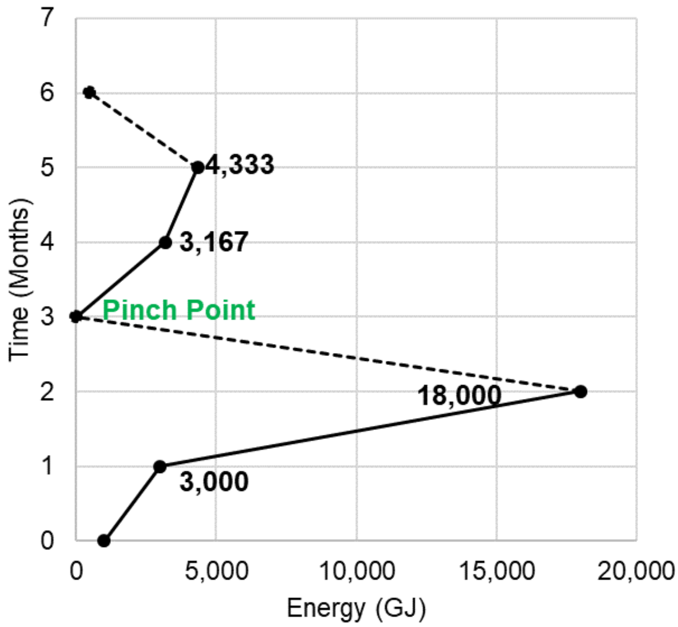
Figure 4.7: Location and distance of the assessed case study. The red dot represents the treatment plant location

4.2.4 Results and Discussion

Figure 4.8 shows the identified production rate and inventory by Pinch Analysis with the consideration of the supply and demand availability. The fixed production rate is identified as 22,000 GJ/month. It can be decreased (adapted) to 6,167 GJ/month after the Pinch Point to minimise the bio-oil inventory. The workforce and number of hired are reduced accordingly. Another option of production rate after Pinch Point is 9,067 GJ/month (with the surplus product/utility), where all the available biomass supply would be processed (Figure 4.9) if there is a possible additional demand (e.g. non bio-oil to energy purpose).



(a)



(b)

Figure 4.8: (a) Composite Curves of demand and production rate and (b) the Grand Composite Curve showing product (bio-oil) inventory

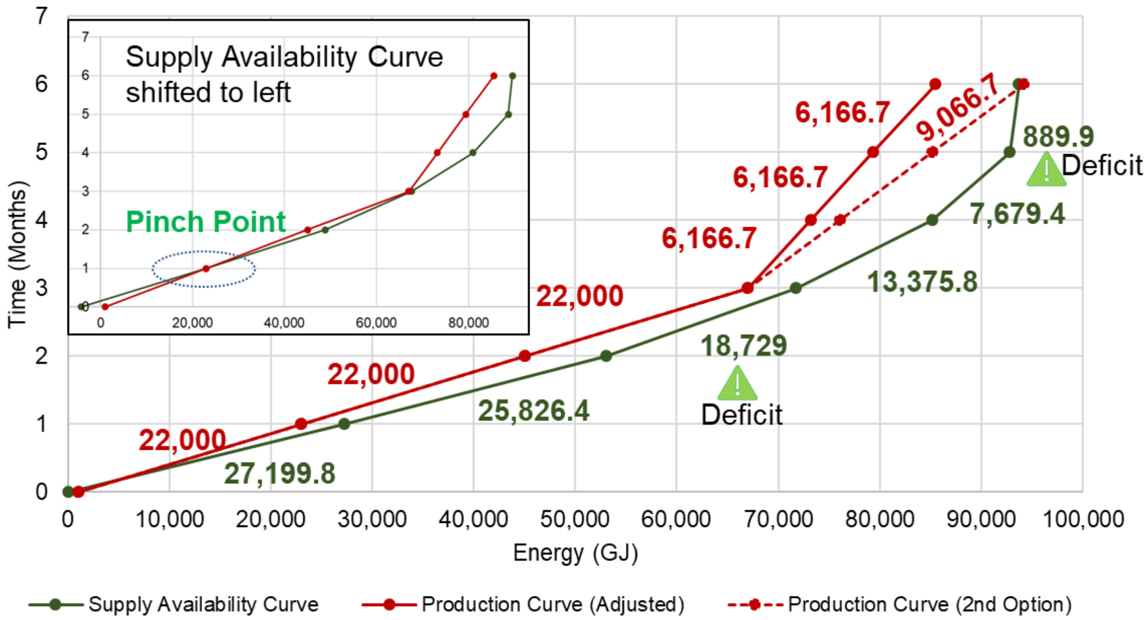
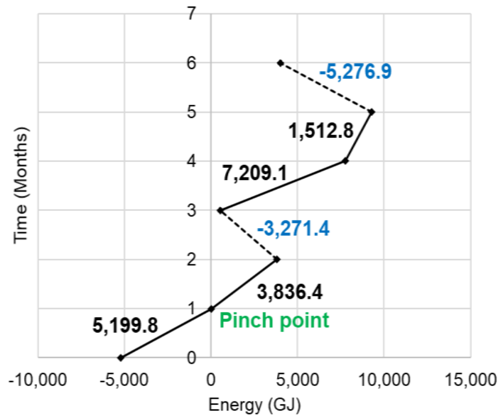


Figure 4.9: Composite Curves of production and available supply.

By referring to the Supply Availability Curve (Figure 4.9), the biomass supply is generally higher than the production rate. However, there is a surplus or deficit at each time interval, as shown in the Grand Composite Curve in Figure 4.10. Biomass storage is required to overcome the deficit on Month 3 and 6. The identified values are 3,271.4 GJ (302 t) on

Month 2, 3,764.1 GJ (301 t) on Month 4 and 1,512.8 GJ (138 t) on Month 5. Different network flow and source can be chosen to obtain the required biomass supply for energy conversion. Eq(4.2) is applied to obtain the flow with the lowest emission and transporting cost, as illustrated in Figure 4.11. For example: 3 biomass sources (S4 = 100 t, S5 = 500 t, S6 = 500 t) are available in Month 4; the selected sources are S5 = 500 t, S6 = 295 t (Figure 4.11) with the optimised cost of 3,581 € (0.36 €/t, Month 4). The average cost for 6 months is 0.51 €/t (43,253 €).



Month	Available Supply (GJ)	Required Supply (GJ) based on Production Curve	Storage (GJ)
1	27,199.8	23,000.0	0
2	25,826.4	23,000.0	3,271.4
3	18,729.0	23,000.0	Deficit
4	13,375.8	6,166.7	3,764.1
5	7,679.4	6,166.7	1,512.8
6	889.9	6,166.7	Deficit
Storage required to overcome the deficit on Month 3 and 6			

Figure 4.10: The Grand Composite Curve showing excessive and deficit biomass availability as well as the identified required supply. Value in blue font (at negative gradient) indicates the deficit at that time interval.

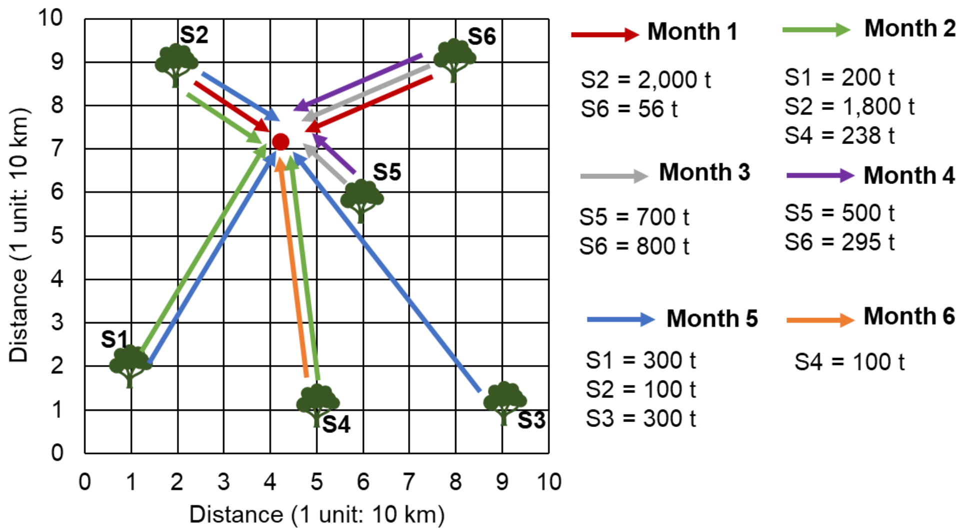


Figure 4.11: The biomass flow in each time intervals (Month) to fulfil the demand, considering the required inventory and storage

4.2.5 Conclusion

The applicability of Pinch Analysis in production, inventory and storage planning has been demonstrated. Results of the case study suggest a production rate of 22,000 GJ/month (Month 1 - 3) and 6,167 GJ/month (Month 4 - 6). To fulfil a total energy demand of 85,000 GJ, which does not distribute evenly across the month, inventory (Month 1 = 3,000 GJ; Month 2 = 18,000 GJ; Month 4 = 3,167 GJ; Month 5 = 4,333 GJ) is needed. Biomass storage of 302 t on Month 2, 301 t on Month 4 and 138 t on Month 5 are required to overcome the deficit on Month 3 and 6. The biomass flow (sourcing/allocation) is optimised for the lowest emission and transporting cost solution, suggesting 0.51 €/t. This simple heuristic method is relatively easier to understand for production planning with seasonal supply and demand. It can be even further extended as this methodology offers the room for the inclusion of social preferences to the planning. Consideration of biomass degradation during the holding time, the inclusion of a wider range of transportation mode, the transfer station, pre-treatments and scheduling are going to be developed in a future study.

CHAPTER 5

P-GRAPH TO ASSESS THE WASTE MANAGEMENT SYSTEM

5.1 Application to Waste Treatment System

The work presented in this section is based on the author publication submitted to Science of Total Environment entitled "Implementing Circular Economy in Municipal Solid Waste Treatment System using P-Graph", as clarified on Page V (Contributing publication). The author of this thesis is the first and corresponding author of this publication. The other co-authors who contributed to this publication are the supervisor Prof Klemeš, Dr Walmsley and Dr Bertók, where none of them is a student. My original contributions are listed in the introduction.

5.1.1 Introduction

Circular Economy (CE) has risen in popularity in recent years as a conceptual model to guide better use of natural resources and management of waste (Murray et al., 2017). The model has proven useful in the field of Waste-to-Energy (Pan et al., 2015) as a means extract value of waste, minimising the consumption of fossil fuels. However, overemphasis on a completely closed-cycle economy and a general lack of understanding physical laws (e.g. thermodynamics) has led to criticism of CE (Skene, 2018). Although many of the points are valid, the CE still provides an important transition vector for the world's economy. Engineering methods and tools, e.g. Process Integration, Pinch Analysis (Klemeš et al., 2018), and P-graph (Bertók and Bartos, 2018), which traditionally have not been linked to CE, can form a technical foundation from which to embed sustainability and CE into system design through the framework of Circular Integration (Walmsley et al., 2019). One of the linchpins for closing the CE loop is minimising the waste flow out from the system, both the waste materials (material loop) and the emissions (ecology loop). Waste management planning still one of the world's most substantial and critical management challenges for emission reduction. The current paper focuses on the integrated treatment of municipal waste to recover valuable products that offset the release of harmful emissions and pollution as well as reduces the input of virgin materials, including fossil fuels, into the broader economy.

Industrialised nations with high economic standards, urban expansion and technological development contribute to increasing Municipal Solid Waste (MSW) generation. The waste generation incurs costs for its collection, treatment and disposal as well as contributes to environmental issues such as greenhouse gas (GHG) emission and air, ground and water pollution. Maalouf and El-Fadel (2019) emphasised the need to improve the accounting practice for emissions from waste management to more accurately reflect reality. The compositions and characteristics of MSW vary for different cities, countries and regions. An adequate design of waste management systems highly depends on the waste amount, its composition (Ghienea et al., 2016), and the current waste separation practices. Waste to Energy (WtE) conversion is one of the possible waste treatment approaches to supply energy and support continuing economic growth and industrial development. Various approaches have been applied to identify suitable waste treatment options and management systems. de Souza Melaré et al. (2017) reviewed the possible approaches, dividing them into heuristic methods, multi-criteria decision analysis, graphs and network theory, mathematical optimisation, stochastic process techniques, and statistical methods. Each of the approaches has its own strength and weakness, as reviewed by Cobo et al. (2018). There is no absolute best approach where the suitability is subjected to the type and size of the problem as well as the primary goal (e.g. heuristic methods not necessarily providing an optimal solution). Mathematical programming and material flow analysis with the support of system assessment tools (e.g. life cycle assessment) is recommended by Cobo et al. (2018) to the design of circular integrated waste management system. However, mathematical programming requires a certain level of knowledge for understanding which might not be equipped by all the practitioners/ stakeholder. Environmental sustainability is not the main accounting concern of material flow analysis as a high recycling rate (use of secondary materials) does not necessary, reflecting a low environmental footprint.

Chatzouridis and Komilis (2012) applied binary programming to optimise MSW management and transfer systems in terms of minimising cost. Chifari et al. (2017) analysed the cost of municipal waste management in Japan by dividing the problem into the collection, processing, and disposal. The empirical results concluded the separate collection of recyclable portions reduces processing cost at intermediate treatment facilities, but not the overall waste management cost. Economopoulos (2010) assessed the techno-economic aspects of mechanical biological (bio-drying, anaerobic, aerobic), and thermal treatment processes (incineration, gasification, pyrolysis). Their analysis identified aerobic mechanical biological treatment as being the most economical and least capital-intensive treatment approach for MSW. A circular system (waste recovery) has to be both economically and environmentally sustainable.

Environmental impacts have started to receive considerable attention with the growing concern on sustainability. Li and Huang (2010) state that the inclusion of environmental impacts can alter the traditional waste allocation pattern. Life cycle assessment (LCA) is commonly applied to identify waste management and treatment systems with minimum environmental impacts. Vadenbo et al. (2018) analysed the environmentally friendly strategies in managing biomass/agricultural waste. They deemed the deployment of bioenergy from wood and manure as environmentally favourable in contrast to the substrate that could be used as animal feed. Liu et al. (2017) assessed four different garbage treatment systems for Beijing using an emergy-based LCA approach, which attempts to quantify all impacts in a single standard emergy unit; however, emergy calculations often do not correlate well to economics. Leme et al. (2014) conducted a comprehensive study, assessing the environmental and economic components of MSW of individual treatment approaches. Sun et al. (2018) assessed the efficiency of the energy recovery of MSW by integrating different treatment systems and quantifying the energy recovery performance and CO_2 emission reduction. The results of the cost-benefit analysis align with the highest energy recovery efficiency option but do not attain the highest GHG emissions reduction option.

Few studies have conducted a combined cost and environmental optimisation, mainly due to the uncertainty in combining multiple criteria. Levis et al. (2014) formulated a generalised solid waste optimisation life-cycle framework to enable multi-period optimisation of MSW management. A strength of this framework is its ability to respond to future changes in pricing, e.g. operational and energy cost, environmental impacts, and associated policies. The aggregation of results from economic and environmental assessments can also result in the loss of valuable information (Soltani et al., 2017). In contrast, a multicriteria assessment highly depends on the allocation of subjective weighting factors (Arikan et al., 2017). A weighting system is unavoidable when different criteria need consideration. Mirdar Harijani et al. (2017) set an objective function including economic, environmental and social components for their proposed model of MSW pre-treatment stage, i.e. recycling. Environmental impact can be expressed as an externality cost (Ao, 2017). Kim and Jeong (2017) assessed the recovery options for industrial waste to achieve minimum economic and environmental costs. Vadenbo et al. (2014) similarly proposed a multiobjective mixed-integer linear programming optimisation model for waste and resources management for industrial networks. However, in each case, the focus on the optimum solution while near-optimal solutions are overlooked.

Cost-effective and environmentally friendly resource management is essential to achieve waste as a secondary resource concept and operationalising the CE concept. A comprehensive assessment framework, supported by appropriate engineering tools, can assist the integrated design and selection of MSW treatment operations. One such process engineering tool is P-graph (P-graph Studio, 2018), which is a combinatorial optimisation framework for Process Network Synthesis (PNS) problems (Friedler et al., 1996). The aim of this study is to develop and demonstrate the applicability of P-graph for an integrated design of waste management systems in support of a CE. The developed P-graph framework identifies the suitable treatment approaches for a MSW system by considering the economic balance between the main operating cost, type, yield, quality of products, as well as GHG emission (as an externality cost). Four different types of MSW composition grouped by country income level are assessed. A three-layer maximal structure consists of different types of waste separation, waste treatment approaches and products (energy, nutrient sources) are presented. The impacts of altering the price of biofuel, digestate, compost, GHG, as well as electricity and heat to the suggested integrated treatment structure is investigated. This provides a broader perspective on the suggested MSW system structure, as the prices of products and utility depend on the demand and resources at each place and often change with time. **My novel contributions are**:

(i) The demonstration and application of P-graph as a potential optimisation tool in proposing a suitable waste management system that progresses the CE concept.

(ii) An optimisation procedure that can scale to consider the integration of multiple treatment solutions (instead of limiting the solution to a single waste treatment technology).

(iii) The identification of both optimal and near-optimal solutions for MSW systems to develop a set of options that can be further analysed for practicality, safety, and other factors that are difficult to embed into a mathematical model.

(iv) The analysis of linking income level to waste composition and optimal waste utilisation structure as demonstrated through a case study, considering both burdening and unburdening GHG emissions.

5.1.2 Method

A waste treatment structure is developed in P-graph to assess the following sets of analysis:

(i) To investigate a set of optimal treatment pathways/waste management system from the economic and environmental (GHGs expressed in externality cost) perspectives of four different MSW composition,

(ii) To analyse the differences in the optimal system structure with and without the consideration of GHG credits, and,

(iii) To examine the sensitivity of the optimal structure under different product and utility prices.

The objective function of the optimisation is to maximise profit (P) as defined in Eq(5.1):

$$\max P, \text{ where } P = A_{ghg}C + MV_{pu} - OC - E_{ghg}C \quad (5.1)$$

where $A_{ghg}C$ is the credit of avoided GHG emission from the recovery product/utility. It is estimated by multiplying the amount of recovered product/utility with the emission factors of displacement and the GHG pricing. For example, the amount of electricity multiplies the emission factor of conventional electricity production (the displacement) and GHG pricing; the amount of nitrogen in the compost multiply by the emission factor of nitrogen fertiliser production (the displacement) and GHG pricing. MV_{pu} is the market value of the product/utility recover from the treatments, OC is the operating cost of waste treatments, $E_{ghg}C$ is the penalty of GHG emission during the treatment process. The reported unit is in € (Euros).

Figure 5.1 shows a general example of P-graph structure for an MSW system optimisation. The waste is collected, separated (Layer 1) into different fractions and transported to different waste utilisation and treatment options. The treatments (Layer 2) incur the operating cost and release emission. The recovered products can have different utilisation, market value and the credit of avoided emission (Layer 3).

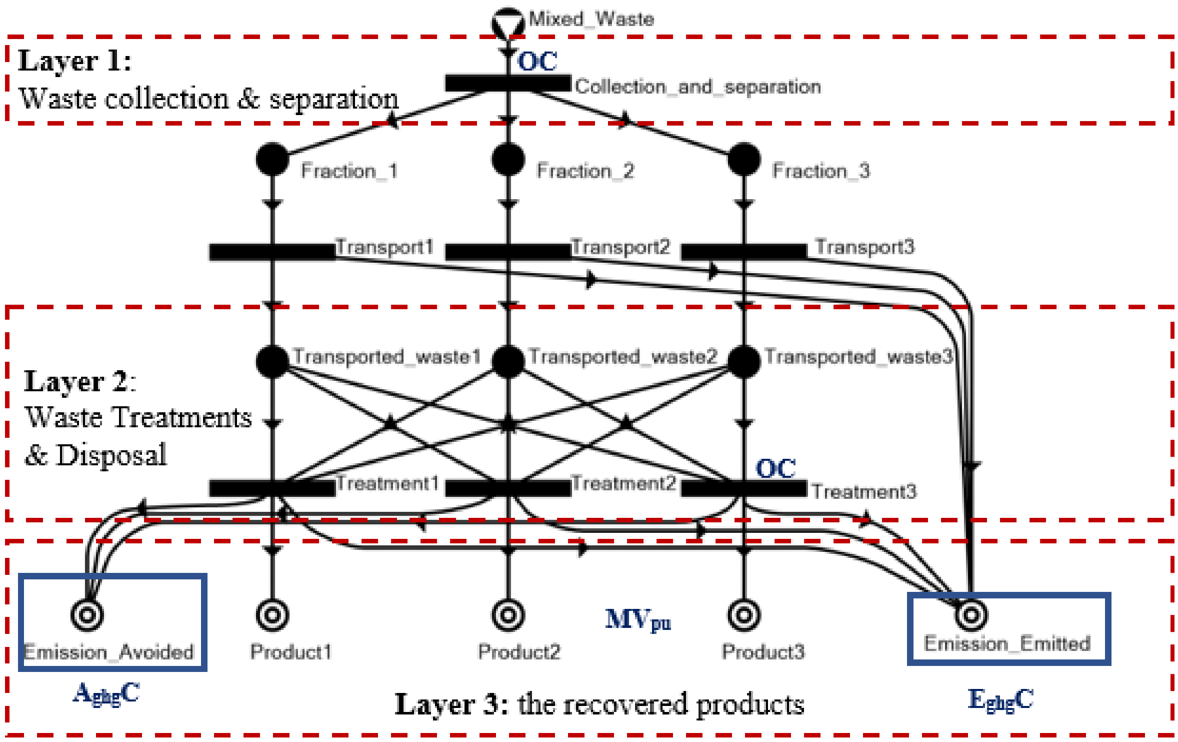


Figure 5.1: The generic waste management model using P-graph

5.1.3 Case Study

A case study was conducted to identify the most suitable waste treatment approaches for four scenarios in demonstrating the effectiveness of developed P-graph structure to the waste management system design. Table 5.1 shows the four assessed scenarios based on differing compositions. The composition of the MSW is according to the income level (low, low-middle, upper-middle and high) as categorised in UNEP (2015). The division of income levels is defined using gross national income per capita in USD. The waste treatment approaches are identified by considering the economic balance between the main operating cost, type, yield, quality of products, as well as the GHG emission (as an externality cost).

Figure 5.2 shows the developed waste treatment structure for this case study. In Figure 5.2, the operating unit (rectangular box) and intermediate in black colour that without a label are the dummy process (change of unit or platform for combination). RM1_U and RM_U are recycling material in different quality. The wet AD is assumed to be located in the Mechanical Biological Treatment (MBT) plant, sorting facility with a form of biological treatment. The dry AD is located away from the MBT; the feedstock is the processed waste (bio-drying) from MBT.

Table 5.1: Composition (UNEP, 2015) and pre-treatment of MSW

	Composition 1	**Composition 2**	**Composition 3**	**Composition 4**
Income Economies	Low ≤ 1,035 USD (~≤ 903 €)	Low-Middle 1,036 - 4,085 USD (~904 - 3,563 €)	Upper-Middle 4,086 - 12,615 USD (~3,564 - 11,003 €)	High ≥12,615 USD (~≥11,003 €)
Composition of MSW	Organic & Paper=53 & 6% Plastics= 7% Glass=2% Metals= 2% Textiles =2% [a]Other=28%	Organic & Paper=53 & 11% Plastics= 9% Glass=3% Metals= 3% Textiles =3% [a]Other=18%	Organic & Paper=46 & 19% Plastics= 12% Glass=5% Metals= 4% Textiles =3% [a]Other=11%	Organic & Paper=34 & 24% Plastics= 11% Glass=6% Metals= 5% Textiles =1% [a]Other=19%
Pre-treatment/ separation (Layer 1)				
Minimum separation[b]	66% Incinerable 4% Recyclable (2% Glass+ 2% Metals) 30% Landfill	73% Incinerable 6% Recyclable 21% Landfill	77% Incinerable 9% Recyclable 14% Landfill	69% Incinerable 11% Recyclable 20% Landfill
At source separation[c]	59% AD or Composting **and** 7% Incineration + 30% Landfill + 4% Recyclable **or** 37% Landfill + 4% Recyclable	64% AD or Composting **and** 9% Incineration + 21% Landfill + 6% Recyclable **or** 30% Landfill + 6% Recyclable	65% AD or Composting **and** 12% Incineration + 14% Landfill + 9% Recyclable **or** 26% Landfill + 9% Recyclable	58% AD or Composting **and** 11% Incineration + 20% Landfill + 11% Recyclable **or** 31% Landfill + 11% Recyclable
MBT[d]	11% Recyclable 16% Landfill **and** 73 % Incineration **or** 59% AD + 14% Landfill	15% Recyclable 12% Landfill **and** 73 % Incineration **or** 64% AD + 9% Landfill	21% Recyclable 8.5% Landfill **and** 70.5% Incineration **or** 65% AD + 5.5% Landfill	22% Recyclable 9.5% Landfill **and** 68.5% Incineration **or** 58% AD + 10.5% Landfill

Table description: The purple line/arc is a symbol of flow, showing the insertion of input data in the P-graph structure, see description in Section 2. [a]Assume all the "Other" have to send to the landfill. For MBT, assume 50 % of the "Other" can be sent to incineration. [b]The organic proportion is not separated, but the recyclable (glass and metal) are separated. [c]Organic and recyclable (glass and metal) proportion are separated. [d]Intensive sorting- the proportion of recyclable are more detailed (e.g. plastic), and the quality/price of the recycled material is higher), the organic proportion is separated. [d]Cost= [27.5 USD/t] 23.33 EUR/t. The emission of the pre-process of MSW (MBT and recycling process-layer 1) is assumed to be zero and at no cost.

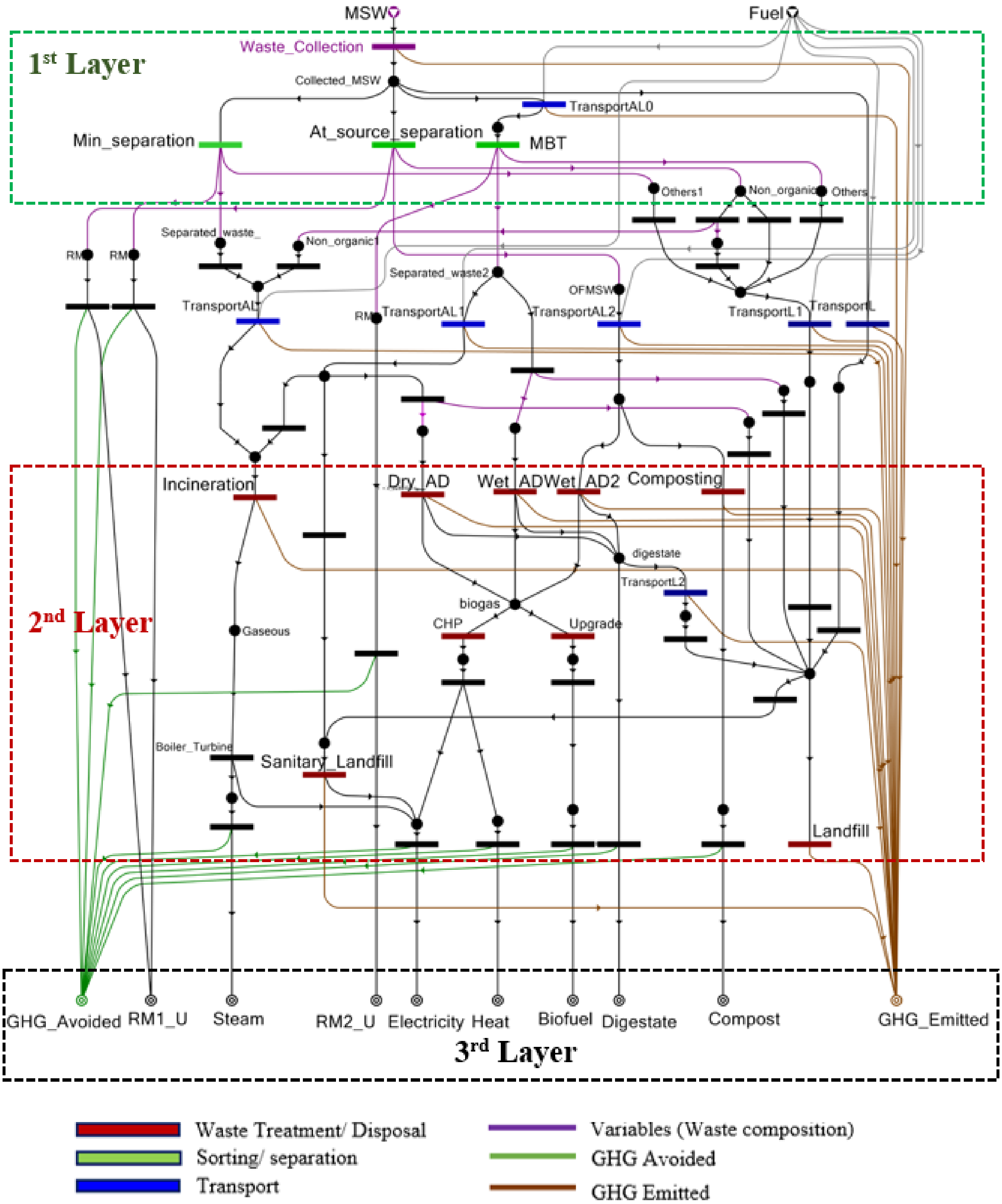


Figure 5.2: The complete waste treatment structure used in the case study.

The first layer has three sorting and separation techniques: mechanical biological treatment (MBT), minimum separation, at source separation. The second layer is different treatment and disposal methods (incineration, anaerobic digestion (AD), composting, sanitary landfill, landfill and recycling). The third layer consists of various types of products, including electricity, heat, recycle materials, biofuel, digestate, compost, as well as the GHG emitted and avoided. The purple curves are the variables where the data inputs would change according to the waste composition of the different scenarios, as stated in Table 5.1.

In this study, the MSW pre-treatment and separation processes (Layer 1) include minimum separation, at source separation and mechanical biological treatment (MBT). Of these, MBT is the most intensive sorting operation. The waste amount of all scenarios is set at 500,000 t/y following the study of Chefdebien (2016), and the focus is on the synthesis and integration of waste treatment and utilisation operations that produce the highest profit (or minimum cost). The distance to the treatment plants and between different treatment plants are assumed to be same, set as 10 km, i.e. from the source to the AD plant is 10 km and from the AD plant to the landfill is another 10 km. Waste collection has not been fully considered in this study with the assumption that it needs to be collected regardless of the type of treatment. The influence on waste treatment selection is low. However, this factor should not be disregard. Waste collection is included in the proposed model, but in performing the case study, the value is set as 0 as localised input data are needed. To demonstrate the importance of waste collection in the overall profit or operating cost of waste management, the model implements an estimated general waste collection fees based on the situation in countries with different income level as reported by UNEP (2015).

Tables 5.2, 5.3 and 5.4 present the input data applied in the case study. Table 5.2 presents the operating cost and GHG emission factors of different treatment approaches. Table 5.3a shows the amount of recovered products and utility as well as the amount of potential avoided emission. Table 5.3b shows the potential value of recovered products and utility as well as mitigated emission. Table 5.4 shows the waste transportation parameters.

Table 5.2: Data input for Layer 2- the treatment approaches

Treatment Approaches (Layer 2)			
Treatments	Data	Reference	P-graph Symbol
Incineration			
Operating cost[a]	81.47 €/t	UNEP (2015)	
GHG emitted	386 kg CO_{2eq} /t	Thinkstep AG (2017)	
AD			
Operating cost[a]	51.45 €/t	UNEP (2015)	
Additional operating cost- CHP	0.015 €/t	Wu et al. (2016)	

Additional operating cost-biofuel upgrading	0.189 €/t	Larsson et al. (2015)	
GHG emitted	228.5 kg CO_{2eq} /t	Phong (2012)	
Composting (Windrow)			
Operating cost[a]	36.45 €/t	UNEP (2015)	
GHG emitted	26.3 kg CO_{2eq} /t	Thinkstep AG (2017)	
Sanitary Landfill			
Operating cost[a]	34.3 €/t	UNEP (2015)	
GHG emitted	0.631 kg CO_{2eq} /t	Thinkstep AG (2017)	
Landfill			
Operating cost[a]	5.57 €/t	UNEP (2015)	
GHG emitted	568 kg CO_{2eq} /t	Ritchie and Smith (2009)	

P-graph Symbol serves as a guideline for locating the P-graph components. Red rectangular is the operating unit of Layer 2. Brown line/arc is the GHG emitted flow (performance ratio). Further illustrated/described in Section 5.1.2. [a]The estimation is for comparative purposes and not indicating the actual cost.

Table 5.3a: Data input for Layer 3- The value and avoided emissions of the products

Amount of Utility/Product/Emission (Layer 3)			
Utility/Product/Emission	Data	Reference	P-graph Symbol
Incineration			
Amount of electricity	315 kWh/t	Thinkstep AG (2017)	
Amount of heat	795 kWh/t	Thinkstep AG (2017)	
AD			
Amount of biogas	150 m^3/t	Getahun et al. (2014)	
Amount of digestate	0.9 t/t; 0.01 % N	Fan et al. (2018b); Annachhatre (2012)	
Amount of electricity	1.81 kWh/m^3 biogas	Wu et al. (2016)	
Amount of heat	2.27 kWh/m^3 biogas	Wu et al. (2016)	
Amount of biofuel	6.37 kWh/m^3 biogas	Larsson et al. (2015)	
Composting			
Amount of compost	600 kg/t (0.03 t N/t)	Fan et al. (2018c)	
Sanitary landfill			
Amount of electricity	0.0813 kWh/t	Thinkstep AG (2017)	

Avoided emission			
Avoided emission from electricity produced	0.5 kg CO_{2eq} /kWh	Thinkstep AG (2017)	
Avoided emission from heat produced	0.0689 kg CO_{2eq} /kWh	Thinkstep AG (2017)	
Avoided emission from biofuel produced	0.25 kg CO_{2eq} /kWh	Thinkstep AG (2017) (based on diesel emission)	
Avoided emission from fertiliser/ nutrient produced	3,600 kg CO_{2eq} / t N	Yara HESQ (2014)	
Avoided emission from recovered recycle material 1[a]	0.285 kg CO_{2eq} /t	Assumed based on US EPA (2018)	
Avoided emission from recovered recycle material 2[b]	0.3725 kg CO_{2eq} /t	Assumed based on US EPA (2018)	

P-graph Symbol serves as a guideline for locating the P-graph components. Black line/arc is the product amount flow (performance ratio). Green line/arc is the GHG emission avoided flow (performance ratio). Further illustrated/described in Section 5.1.2, Figures 5.1 and 5.2.

Table 5.3b: Data input for Layer 3- the potential value of recovered products/utility and emission

Value of Utility/Product/ Emission (Layer 3)			
Product/Utility/ Emission	Data	Reference	P-graph Symbol
Electricity	0.14 €/kWh	Wu et al. (2016)	
Heat	0.04 €/kWh	Wu et al. (2016)	
Biofuel	0.119 €/kWh	Larsson et al. (2015)	
Digestate	1.81 €/t	De Clercq et al. (2017)	
Compost	3.81 €/t	Meyer-Kohlstock et al. (2015)	
Recycle material 1	25.5 €/t	Eurostat (2018)	
Recycle material 2	163.25 €/t	Eurostat (2018)	
GHG emitted	-0.0174 €/ kg CO_{2eq}	World Bank Group (2016)	
GHG avoided	+0.0174 €/ kg CO_{2eq}	World Bank Group (2016)	

P-graph Symbol serves as a guideline for locating the P-graph components. Black circle node refers to the recovered products/utility. Brown circle node is the emitted GHG and green circle node is the avoided GHG. Further illustrated/described in Section 5.1.2, Figures 5.1 and 5.2.

Table 5.4: Data input of waste transportation

Waste Transportation	Data	Reference	P-graph Symbol
Fuel consumption	1.083 kWh/tkm	Pöschl et al. (2010)	
Cost of diesel	0.2 €/kWh	NSW (2016)	
GHG Emitted	0.25 kg CO_{2eq} / kWh	NEF (2017)	

P-graph Symbol serves as a guideline for locating the P-graph components. Further illustrated/described in Section 5.1.2 and Figures 5.1 and 5.2.

As supplementary materials, Figure S1 shows the data input column of P-graph software for raw material , operating unit , intermediate , product and flow/performance ratio (connecting line/arc). An example for each of the P-graph components is illustrated. The examples cover MSW, incineration, non-organic, GHG emitted, and electricity, as stated in the bracket, see Figure S1. This is to provide the reader with an idea of the available functions of P-graph and serve as a simple guideline. The variation of investment cost is not considered in this case study. This study focuses on operational expenditure. It can be considered if the data is available, see Figure S1b. See Bertók and Heck (2016) for the further details on the P-graph software.

The required flow ("Req. flow"), in Figure S1d, of GHG emitted (i.e. the brown product node in Figure 5.2) is set to 1 t/y (extremely low), which forces the MSW to be processed even if it achieves no profit (axiom 1). In this case, P-graph will suggest solutions with a minimum loss, which in this case study required all available waste to be processed. A minimum GHG emitted flow was set since it must be present in all solutions, i.e. cannot be avoided. To identify the baseline scenario (i.e. all the MSW to the landfill), the capacity multiplier-upper bound (See Figure S1b) of the three separation processes (Green operating unit in Figure S1) is set to 0, preventing their use in any solution and forcing the MSW to be sent to the landfill. Set 2, which analyses the impact of GHG price on the optimal structure, is assessed by altering the price of GHG emitted and avoided to 0 (Figure S2). Figure S3 shows the P-graph interface in illustrating the solutions. P-graph identifies the optimal solution and a set of near-optimal solutions, as requested by user input. The importance of near-optimal solutions in decision support has been previously discussed by Voll et al. (2015).

The identified results (the maximum profit) by the P-graph solver serve as an indicator for the recommended pathway/structure, where a higher value reflects higher feasibility. This demonstration study did not consider a variation of investment, operational (manpower) and maintenance costs. The actual profit can be identified if localised and exact data is collected and applied to the developed structure.

To assess the impacts of altering the price of products/utility (Sensitivity analysis) on the overall results, the price of the biofuel, digestate, compost and GHG (as the data input column display in Figure S1d) is modified by applying 100 % reduction to + 100 % increment (20 % interval). The change in the profit and suggested the integrated structure of treating MSW are evaluated.

5.1.4 Results and Discussion

The results and discussion are divided into three subsections based on the three sets of analysis, as stated in Section 5.1.2.

5.1.4.1 Optimal Treatment Pathways of Different Waste Compositions based on Income Levels

Figure 5.3 shows the optimal structure of Composition 1 (low-income country) by P-graph. The suggested waste treatment structure consists of Layer 1 – at source separation, Layer 2 – recycling, incineration, wet AD, landfill, with Layer 3 – heat, electricity, biofuel, digestate, recycle material. The total GHG emitted (brown lines) is 166,210 tCO_{2eq} and the total GHG avoided (green lines) is 87,493 tCO_{2eq}. This gives a net increase of 78,717 t GHG emitted. By comparison to the baseline scenario with all MSW sent to landfill (See Figure 5.4), the suggested optimal solution avoided 284,000 tCO_{2eq} from landfill and 125 tCO_{2eq} from transporting the waste to the landfill. This result suggests the emission from transportation is comparatively insignificant. This is consistent with the hot-spot analysis by Parkes (2015). The net GHG mitigated (284,125 tCO_{2eq} - 78,717 tCO_{2eq}) is equal to 205,408 tCO_{2eq}. As a ratio, the solution results estimate that 411 $kgCO_{2eq}$ /t of processed MSW is mitigated.

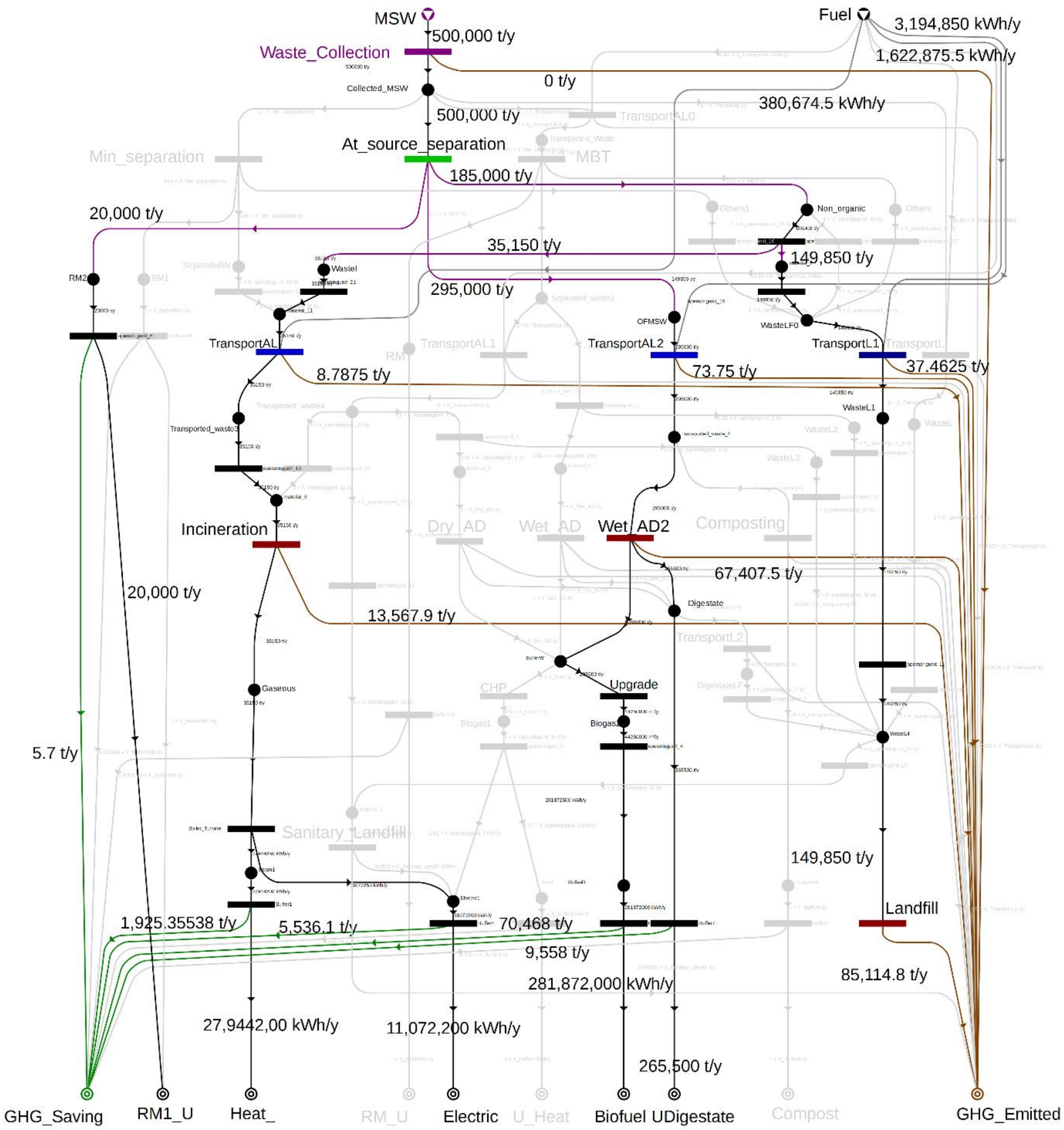


Figure 5.3: The optimal structure of Composition 1.

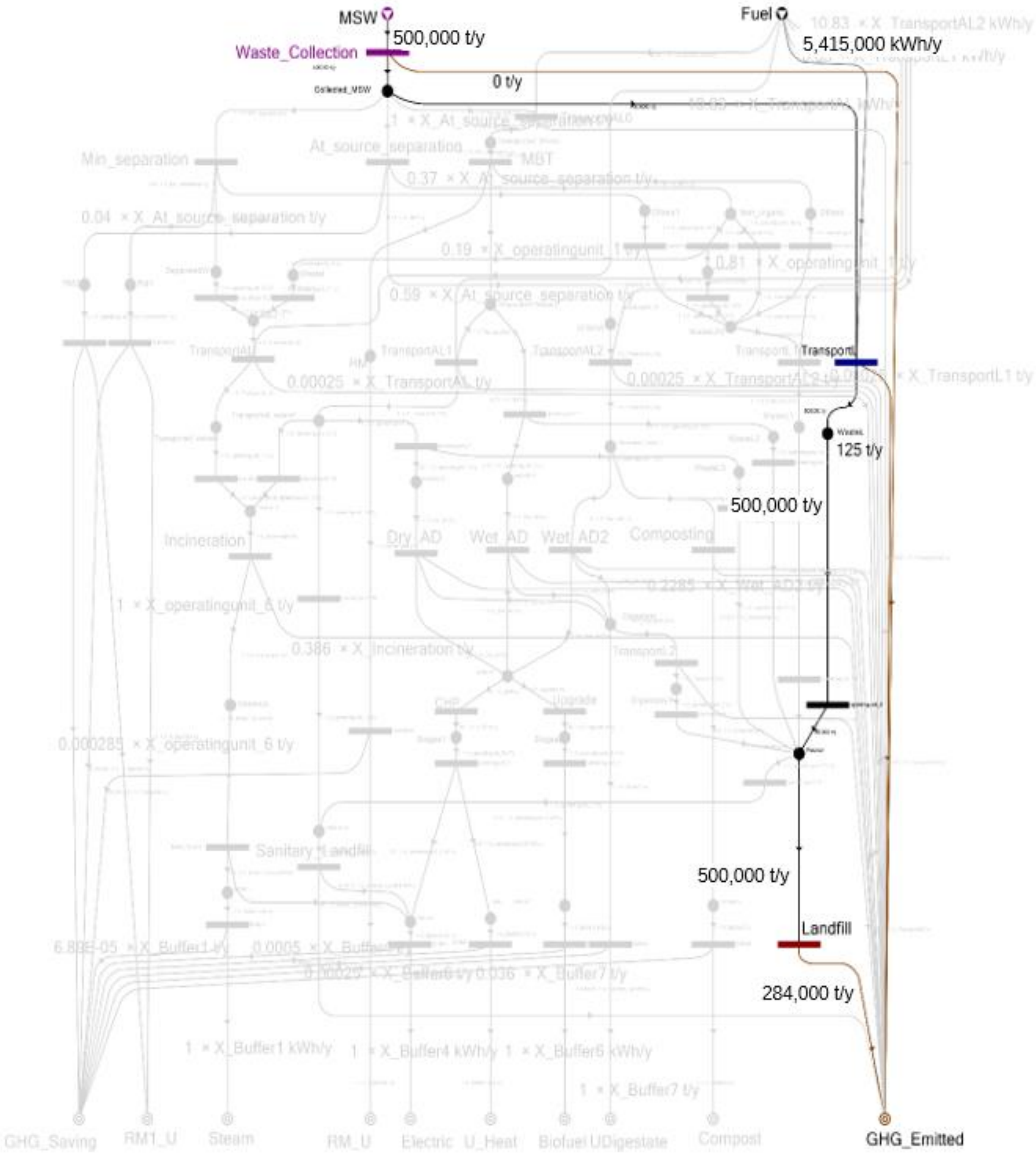


Figure 5.4: The baseline scenario (all the MSW is sent to the landfill)- Composition 1

The breakdown of the cost and profit are not illustrated in the structure in Figures 5.3 and 5.4. The presented data are waste and product flows. The breakdown of overall profit is extracted from the P-graph and illustrated in Figure 5.5 (see the illustration within the blue dotted line). The profit from the product and utility after deducting the treatment operating cost is 18,269,346 € (37 €/t). The potential profit of the suggested optimal waste treatment structure for Composition 1 is 15,860,100 € (32 €/t). Based on Figure 5.5, the GHG externality cost of the optimal solution is -1,369,680 € (-2.7 €/t). The negative value indicated the need for paying the GHG emission. The GHG avoided from the generated products and utility did not compensate for the GHG emission during the treatment process. However, the net GHG emission remains significantly lower than the base case of using a landfill. Compared to the baseline of all MSW sent to landfill, the suggested optimal solution offers an additional 4,943,780 € (10 €/t) profit from the GHG eternality cost. The profit with the inclusion of the avoided emission from the landfill is approximately 20,803,880 €, which equates to a profit of 42 €/t of processed MSW.

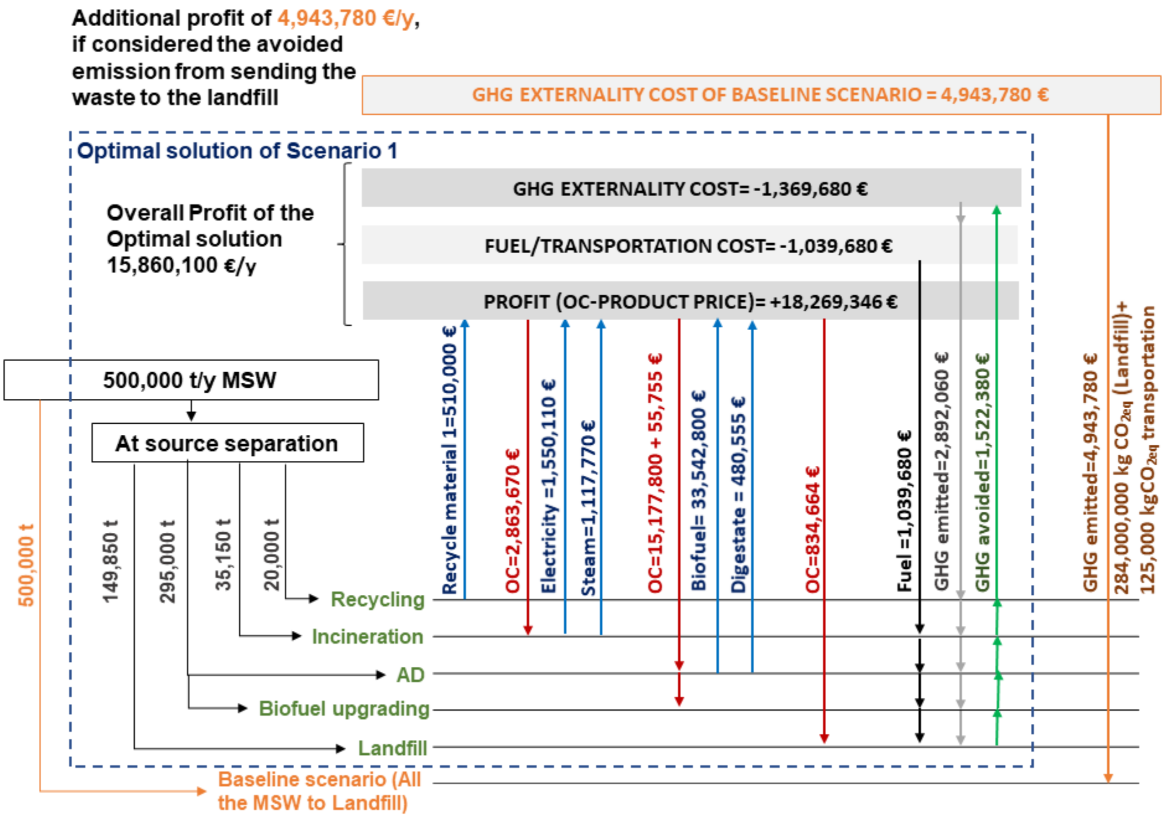


Figure 5.5: The diagram within the blue dotted line is the optimal structure of Composition 1 (as in Figure 5.3) with a detailed cost breakdown. OC=Operating cost.

The other near-optimal structures and the potential profit of Composition 1 are shown in Table 5.5. In contrast to Composition 2 (low-middle income country), MBT is not the first selection for Composition 1. Table 5.6 shows the optimal and other near the optimal structure of Composition 2. The integrated solution consists of MBT, recycling, AD (biofuel, digestate) and landfill offers a potential profit of 18,476,300 €/y (37 €/t). Compositions 3 (24,130,700 €/y or 48 €/t, see Table 5.7) and 4 (22,364,300 €/y or 45 €/t, see Table 5.8) have the same optimal pathway. However, the potential profit is different due to the differences in waste composition and the processing amount of the different waste treatment approach. The 5th feasible solution (near-optimal) of Composition 4, as presented in Table 5.8 is MBT, recycling, AD (biofuel) and landfill. Unlike the other AD solution, it is without digestate. This suggests sending the digestate to landfill instead of using it as a nutrient source for soil is more profitable than the other following solutions. In general, AD treatment to produce biofuel appears as one of the integrated waste treatment solutions for all four compositions. The price of biofuel depends on the technology for implementation and the country policy. The utilisation of biofuel remains low due to the suitability of the conventional engine, which has not been designed to biofuels (Hassan and Kalam, 2013). See Section 5.1.5 for further discussion.

Table 5.5: The optimal and near-optimal solution of Composition 1. Add 4,943,780 €/y (see Figure 5.4) for the overall profit (included the avoided emission from the baseline)

Composition 1 (Low)- The pathway	**€/y**	**€/t**
At source separation, recycling, incineration (heat, electric), wet AD (biofuel, digestate), landfill	15,860,100 (Optimal)	32
At source separation, recycling, wet AD (biofuel, digestate), landfill	15,618,900	31
At source separation, recycling, incineration (heat, electric), wet AD (biofuel, digestate), sanitary landfill	13,036,000	26
MBT, recycling, wet AD (biofuel, digestate), landfill	12,812,400	26
At source separation, recycling, wet AD (biofuel, digestate), sanitary landfill	12,132,500	24

Table 5.6: The optimal and near-optimal solution of Composition 2. Add 4,943,780 €/y (see Figure 5.4) for the overall profit (included the avoided emission from the baseline)

Composition 2 (low-middle**)- The pathway**	**€/y**	**€/t**
MBT, recycling, wet AD (biofuel, digestate), landfill	18,476,300 (Optimal)	37
At source separation, recycling, incineration (electric and heat), wet AD (biofuel, digestate), landfill	18,356,200	37
At source separation, recycling, wet AD (biofuel, digestate), landfill	18,047,500	36
MBT, recycling, dry AD (biofuel, digestate), landfill	17,684,100	35
MBT, recycling, wet AD (biofuel, digestate), sanitary landfill	16,520,100	33

Table 5.7: The optimal and near-optimal solution of Composition 3. Add 4,943,780 €/y (see Figure 5.4) for the overall profit (included the avoided emission from the baseline)

Composition 3 (Upper-middle)- The pathway	**€/ y**	**€/t**
MBT, recycling, Wet AD (biofuel, digestate), landfill	24,130,700 (Optimal)	48
MBT, recycling, Dry AD (biofuel, digestate), landfill	23,365,700	47
MBT, recycling, Wet AD (biofuel, digestate), sanitary landfill	22,798,300	46
MBT, recycling, Dry AD (biofuel, digestate), sanitary landfill	22,033,300	44
At source separation, recycling, incineration (heat, electric), wet AD (biofuel, digestate), landfill	19,504,200	39

Table 5.8: The optimal and near-optimal solution of Composition 4. Add 4,943,780 €/y (see Figure 5.4) for the overall profit (included the avoided emission from the baseline)

Composition 4 (High)- The pathway	**€/ y**	**€/t**
MBT, recycling, Wet AD (biofuel, digestate), landfill	22,364,300 (Optimal)	45
MBT, recycling, Dry AD (biofuel, digestate), landfill	21,620,900	43
MBT, recycling, Wet AD (biofuel, digestate), sanitary landfill	20,500,900	41
MBT, recycling, Dry AD (biofuel, digestate), sanitary landfill	19,757,500	40
MBT, recycling, Wet AD (biofuel), landfill	17,675,800	35

An increase in the income level of the country increases the preference for implementing MBT. This could be explained by the waste composition, which consists of more recyclable materials such as plastic. MBT offers a more acute separation of recyclable materials, e.g. PVC, PP, PT, LDPE, HDPE. MBT has been widely implemented in EU countries (FuturENVIRO, 2017). However, intensifying at source separation practice can avoid the need for MBT. The process of MBT creates a burdening environmental footprint (the MBT process consumes energy) at the same time of mitigating the footprint of the waste. Composting is not selected in any of the cases, although the processing emission is lower, and the avoided emission from fertiliser production is higher. The underlying reason for this non-selection is the product quality, and economic value is low (compost, assumed to contain 3 % of N). The current utilisation and the confidence level of composts for agricultural land remain low.

The waste collection fees have limited attention in this study (input data=0), with the assumption that it needs to be collected regardless of which waste treatment approaches are selected. It is constant and has no influence on the waste treatment structure selection. UNEP (2015) reported the waste collection fees required in different countries based on the income level, see Table 5.9. By considering the service provider to bear the waste collection cost instead of the waste creator (as collection revenue), Composition 1 (low-income country) offers a profit of 870,074 €/y (1.7 €/t), which is significantly lower. There is no profitable solution for Compositions 2, 3 and 4. The developed P-graph waste treatment structure suggest solutions with minimum economic loss. The results highlight the important role of implementing waste collection fees. It ensures the waste to be collected and processed (the service provider) as well as encouraging waste minimisation (the waste creator). Waste management is hardly to be profitable without the government subsidy or the consideration of avoided emission in accounting. The waste generation impacts the environment (availability of land, pollution, health issues) and is hardly profitable without the subsidy or the consideration of avoided emission. This can be further supported by the result illustrates in Figure 5.5.

Table 5.9: The waste collection fees, based on UNEP (2015)

Composition (Country Income Level)	**Waste Collection Cost (€/t)**
1 (Low)	29.98
2 (Low-middle)	44.97
3 (Upper-middle)	55.67
4 (High)	143.47

5.1.4.2 The Impact of GHG Credits

Figure 5.6 illustrated the optimal structure of Composition 1 without setting an externality cost of GHG emission and avoided. Compared to the structure in Figure 5.3, incineration is not chosen. 35,150 t/y of waste is sent to the landfill instead of an AD, the makeup of a total of 185,000 t/y. This suggests the recovered energy and its emission avoided of incineration is not able to compensate the operating and externality costs unless the emission avoided from the landfill is considered. GHG credits play an important role to avoid the landfill option.

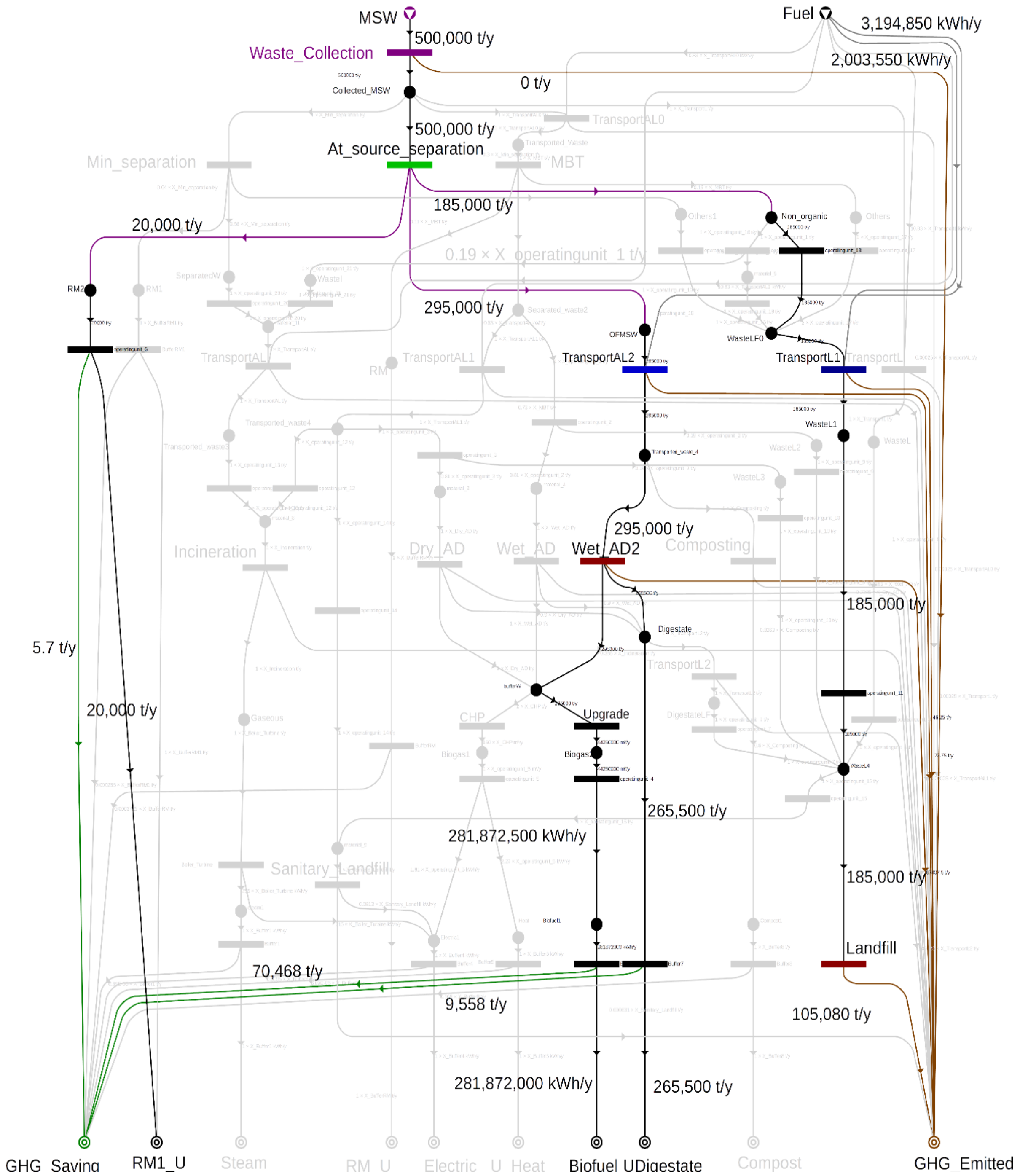


Figure 5.6: The optimal structure of Composition 1 without the consideration of GHG (cost of emission = zero).

5.1.4.3 Sensitivity Analysis: The Impact of Products and Utility Value

Different pricing of the product and utility affect the potential profit, and even the suggested integrated waste treatments. Figure 5.7 shows the changes in structure and profit after altering the cost of biofuel, digestate, compost, GHG, as well as electricity and heat by using Composition 1 as an example. In line with the suggested solutions presented in Tables 5.5 – 5.8, AD process with biofuel production is a must-have treatment in all of the suggested integrated solution. Based on Figure 5.7, the potential profit (blue line/arc) increase with the increase of the biofuel price. The optimal structure remains the same as at source separation, recycling, incineration, AD (biofuel, digestate) and landfill. There is no profitable solution when the price of biofuel is reduced by 60 % (2.8 x 10^6 €/y). The structure with minimum loss is suggested. AD treatment with electricity and heat production is preferable. However, by considering the avoided GHG from landfill (see Figure 5.8), the suggested pathway (AD treatment with electricity and heat production) offers a gain of 2.1 x 10^6 €/y.

The impact of varying the price of compost and digestate on the potential profit is minimal (the changes in profit is small, <1 %). Composting is not selected even if the price of compost increases by 100 % (original price=3.81 €/t). A change in the market prices of electricity and heat impacts the suggested optimal waste treatment structure. However, the change in optimal waste treatment structure only occurs when the prices of electricity and heat fluctuate over 20 %

When there is a 100 % decrease in the price of GHG (i.e. zero cost), the amount of waste that was originally used incineration is now sent to the landfill, in line with Figure 5.5. In contrast to the other products, the increase in GHG pricing, decrease the potential profit (see Figure 5.7). As without considering the emission avoided from landfill, the avoided emission from recovered utility and product is insufficient to cover the emission during the treatment processes. This highlights the potential environmental impact of waste treatment and the importance of waste minimisation. Figure 5.8 shows the changes in overall profit (included the emission avoided from landfill) resulting from the application of different utility, product, and GHG prices.

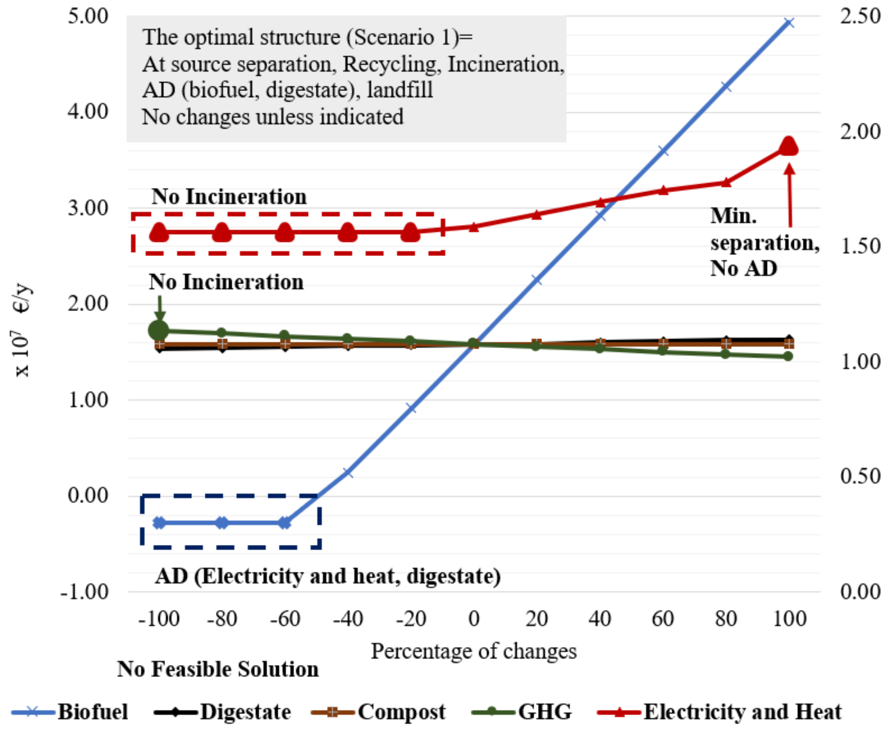


Figure 5.7: The impact of the products and utility cost (-100 % to +100 %) on the potential profit and the suggested optimal solution. The secondary axis (right side, x 10^7 €/y) is for electricity and heat (the red line). Secondary axis is utilised for a better illustration and description, through preventing the line graph lumping together.

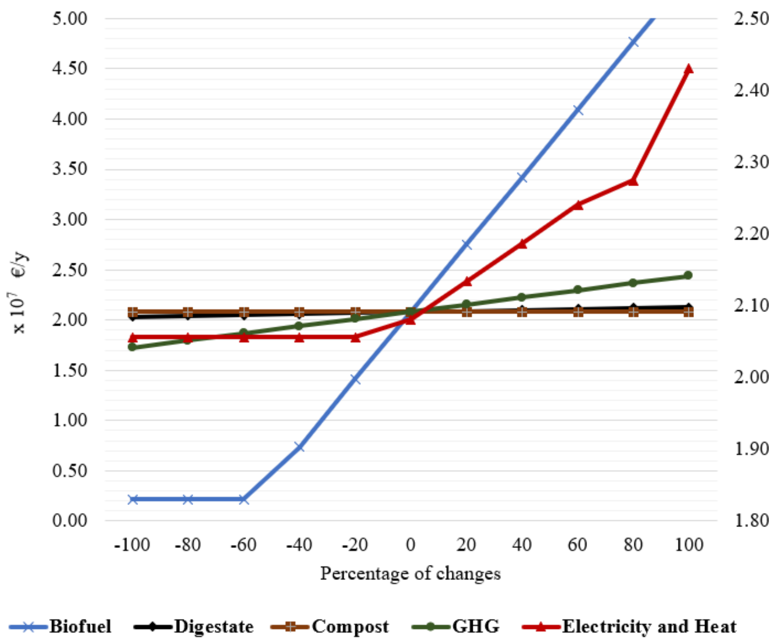


Figure 5.8: The impact of the products and utility cost (-100% to +100%) to the overall profit (considered the baseline scenario-GHG emission avoided from landfill)

5.1.5 Potential Extension and Application of the Developed Structure

The developed model (Figure 5.2) serves as a framework showing the applicability of P-graph by suggesting cost-effective and environmentally friendly waste management systems. It has been applied to a case study considering four MSW compositions based on different country income level. The developed base model by using P-graph methodology has a broader potential and flexibility for extended application. The presented illustrative case study could not capture all the waste management cases and/or reflect the exact feasibility and profit of specific situations, but it can be achieved if the localised data is inputted. The possible extensions include (a) A more detail waste composition. (b) The supply and demand/ industrial symbiosis. (c) Wider parameters and product utilisation.

The waste treatment processes of different MSW fraction have different efficiency and so to the generated output.

(a) Figure 5.9 shows the way to consider the conversion efficiency of the different separated fraction. The specific conversion performance ratio of Incineration 1, 2, 3 for waste fraction 1,2,3 can be inserted.

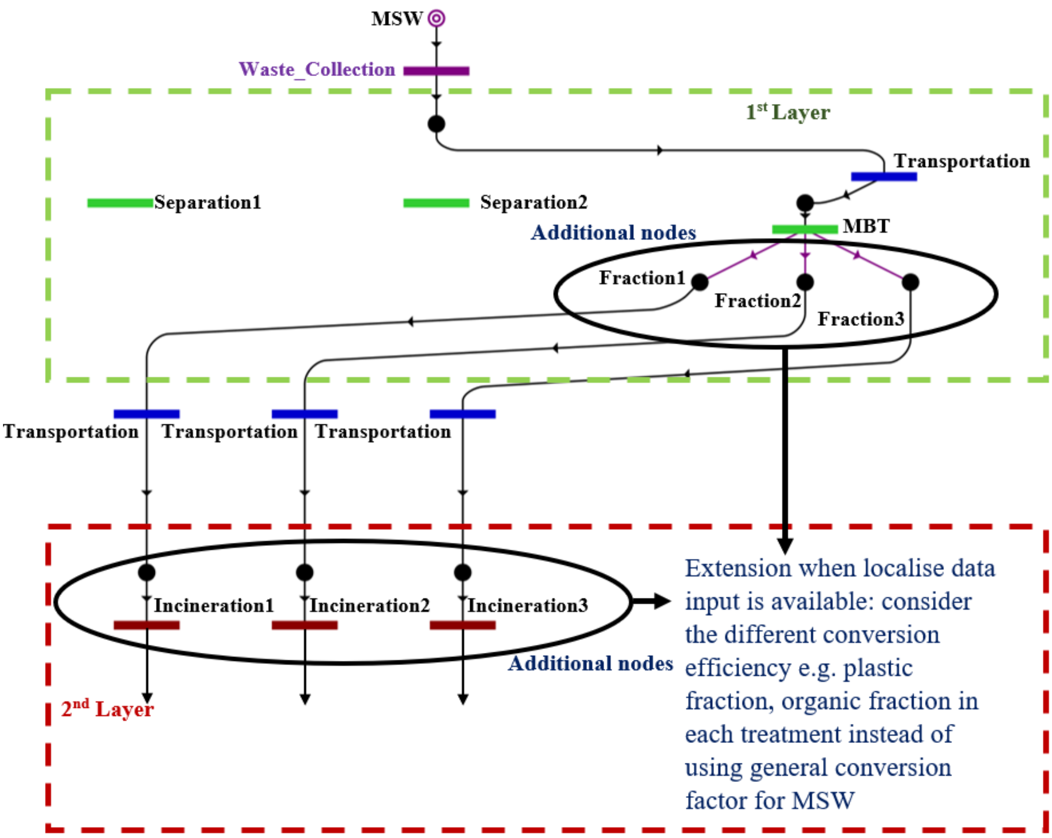


Figure 5.9: Possible extension: a more detail waste composition, using incineration as an example.

(b) The waste of resources (e.g. energy/ compost) can be a waste of resources process if the generated products or utilities are not needed. It is essential to consider the demand at a place. Figure 5.10 shows the example to fix the demand of compost in optimising, another treatment pathway can be selected to process the waste if the demand for compost is fulfil (has to be fulfil = Req flow "demanded value", Max flow "demanded value", should not be more than the demand = Req flow "0", Max flow "demanded value"). To consider industrial symbiosis where utility sharing/ exchange is enabled, by referring to Figure 5.10-3rd layer, the current "product" nodes can be replaced with "intermediate" nodes with additional "operating unit" and new "product" nodes. The new "product" nodes will be the demand of each utility/product at industrial site 1,2,3,4 etc.

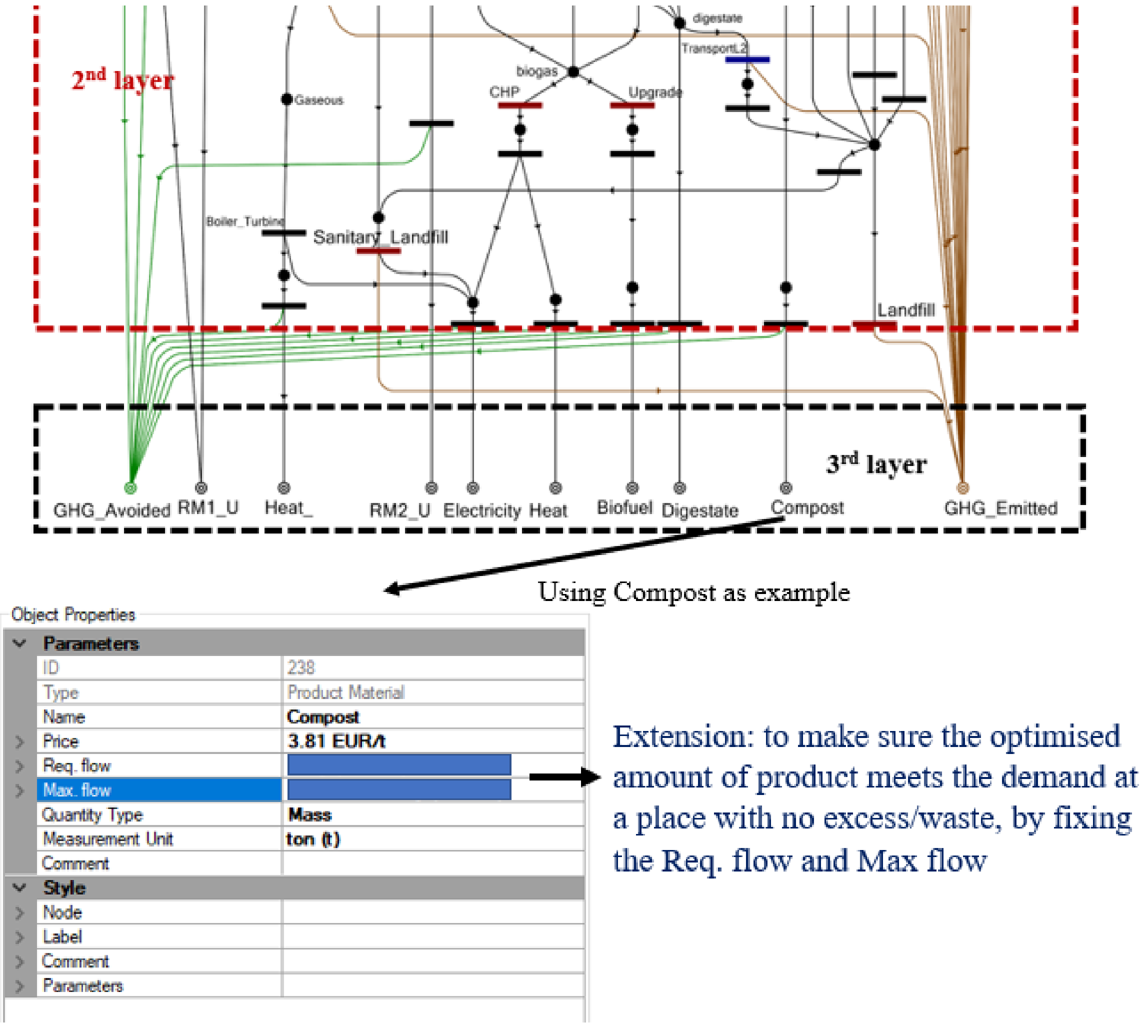


Figure 5.10: Possible extensions: the supply and demand/ industrial symbiosis and broader parameters and production utilisation. See Figure 3 for the complete model structure

(c) The other environmental impacts can be included by adding the “product” node at layer 3 through eco-cost (Vogtländer et al., 2001) or externality cost as performed by Martinez et al. (2017). The presented case study did not take the different utilisation into account. For example, the utilisation of bioenergy for different purposes would lead to different displacement/saving in the GHG emission. The proposed framework can be extended by assessing the secondary bioenergy conversion for residual biofuel, bioethanol, biomethane, solid biofuel, biodiesel, biopetrol as structured by Vadenbo et al. (2017).

5.1.6 Conclusion

The demonstration study underscores the potential application of P-graph to the waste management area to help progress towards a CE. The developed waste treatment structure can be implemented to specific case studies for localised solutions by inputting the relevant data of waste composition, expenditure, capital depreciation, transport distance, emission policy, and product market prices at the targeted area. Additional costs can also be added to the model, where applicable. Near-optimal solutions obtained in P-graph offer a guideline for the stakeholders with conflicting priorities that share the liabilities of MSW and can help achieve mutual agreement on a compromise option. The graphical representation is a strength of the proposed model. It facilitates the understanding for the stakeholders with non-mathematical optimisation background.

For the case study, the treatment solutions suggested for the low-income economy is at source separation, recycling, incineration (heat, electric), wet AD (biofuel, digestate) and landfill. The potential profit of the demonstration case study (Scenario 1) is 15,860,100 €/y (32 €/t). The additional profit from the credit of GHG avoided from landfill is 4,943,780 €/y. As a ratio, the estimated profit is 42 €/t of processed MSW. The GHG mitigated is up to 411 kg CO_{2eq}/t of processed MSW. The potential profit of Scenarios 2, 3, 4 are 18,476,300 €/y (37 €/t), 24,130,700 €/y (48 €/t) and 22,364,300 €/y (45 €/t). The other outcomes that drawn from the case study include: (1) Mechanical biological treatment is suggested instead of at-source separation with the increase of income level. (2) The selling prices of biofuel, electricity and heat have a significant impact on the treatment structure selection compared to compost and digestate product prices. A decrease in the biofuel price by 60 % leads to non-profitable solutions. (3) Changes in the prices of electric and heat by >20 % shifts the optimal solution to select AD instead of incineration. An interesting finding is (4) the low contribution of transportation emission to the total system emissions (including those from the treatment processes).

The proposed P-graph structure can be an effective tool for waste treatment decision-making in CE with low environmental footprints. The main limitation of this study is the case study that has not fully demonstrated the applicability of the proposed structure. Future studies on the application of P-graph to MSW system optimisation could consider a wide scope of inputs and parameters to improve the model's fidelity. This required a bigger and more comprehensive data collection which is currently still a challenge in the field of waste management. Water and nitrogen footprints can be explicitly included and priced instead of limiting the environmental cost to GHG emission alone.

5.2 Application to Pre-and Post-Treatment in Waste Management

The work presented in this section is based on the author's publication in Journal of Environmental Management entitled "Anaerobic Digestion of Lignocellulosic Waste: Environmental Impact and Economic Assessment", as clarified on Page V (Contributing publication). The author of this thesis is the first and corresponding author of this publication. The other co-authors who contributed to this publication are the supervisor (Prof Klemeš), and co-supervisors (Dr Perry and Prof Lee), where none of them is a student. My original contributions are listed in the introduction.

5.2.1 Introduction

Lignocellulosic waste (LW) is abundant in availability and serves as one of the suitable substrates (Vasco-Correa et al., 2018) for the anaerobic digestion (AD). However, it is a complex solid substrate matrix that hinders the hydrolysis stage of anaerobic digestion. The typical composition is 37.5 % cellulose, 22.4 % hemicellulose and 17.6 % lignin (Wyman et al., 2018). Pre-treatments play an important role in improving the process of economics by maximising substrate accessibility to achieve high biogas yield. There are various of pre-treatments that have been introduced in the previous studies, ranging from physical (e.g. mechanical, thermal, irradiation, extrusion, steam explosion), chemical (e.g. alkaline, acid, peroxides, ozonolysis), biological (e.g. enzymatic, fungal, bacteria, consortium) and combined (Fan et al., 2018b).

Zheng et al. (2014) state that there is lacking systematically comparison on the pre-treatments methods of lignocellulosic biomass for biogas production. Various techniques, parameters, performance, advantages and limitation of pre-treatments have been reviewed to fill the stated research gaps. Shafiei et al., (2013) assessed the economic feasibility of steam explosion pre-treatment and identified that the pre-treatment application resulted in 13 % increase in total capital investment but decrease the production cost of methane by 36 %. Cotana et al. (2015) highlight the high operative and investment cost of steam explosion pre-treatment; however, provide a significant environmental benefit which are land usage, carbon emissions and water consumption reduction. Behera et al., (2014) assessed various chemical pre-treatment process and the application at industrial scale. The comparison across chemical, physical and biological treatment is still lacking. The available studies are subjected to limited pre-treatment techniques. Kumar and Murthy (2011) cover a wider range of pre-treatments including dilute acid, dilute alkali, hot water and steam explosion and take in the downstream/post-treatment processing in evaluating the economic performance. However, the process is for ethanol production (ethanol recovery) instead of biogas production. Majority of the assessments are a more focus on cost with a limited discussion on environmental performance. Cost optimal solution is not sustainable without considering the environmental performance.

This study simultaneously assesses the pre-treatment and post-treatments from both perspectives, the cost and the environmental performances (global warming potential, human toxicity, ozone depletion potential, particulate matter, photochemical oxidant creation, acidification and eutrophication potential). Post-treatments determine the quality and utilisation value of biogas. Some of the examples of post-treatment method are pressure water scrubbing, organic-physical scrubbing, amine scrubbing, membrane separation and pressure swing adsorption (Leme et al., 2017). The selection of post-treatment approaches could affect by the demand (utilisation), the composition of biogas, operational cost as well as the regulation/requirement of a country. Different post-treatment subjected to a different level of operational cost and burdening environmental impacts. Li et al. (2017) perform the environmental and economic life cycle assessment of different anaerobic digestion pathways (includes different pre-treatment and post-treatment). The study focusses on physical treatments and is for sewage sludge.

This study aims to evaluate the cost and environmental performance of various pre-treatment and post-treatments of LW for AD. P-graph (P-graph Studio, 2015) is applied to identify the cost-optimal pre-treatment and post-treatment pathways. This optimisation tool has been applied to design sustainable supply chain structures, for example, to design energy supply chain by optimising the cost under sustainability (e.g. ecological footprint) considerations as performed by Vance et al. (2015). This study provides wider options by considering the near cost-optimal solutions in environmental impact assessment using GaBi software (Thinkstep, Germany). This is important as an analysis of the single optimal solution does not provide sufficient information on the robustness of the solution. The practical constraints in the real world could be overlooked, as described by Voll et al. (2015). **My novel contributions are:**

(i) Developed a structure for pre-treatment and post-treatment assessment of anaerobic digestion using P-graph integrated with environmental assessment tool (GaBi)

(ii) Identification of pre-treatment and post-treatments combination with the minimum possible cost incurred and environmental footprints.

(iii) Assess the trade-off between economic and environmental performance by evaluating the optimal and near-optimal solutions.

The contribution of this study has been serving as a performance guideline in selecting the pre-treatment and post-treatment options for LW.

5.2.2 Method

This study assesses the optimal pre-treatment and post-treatment alternatives for anaerobic digestion of LW. Figure 5.11 shows the flow structure of this study.

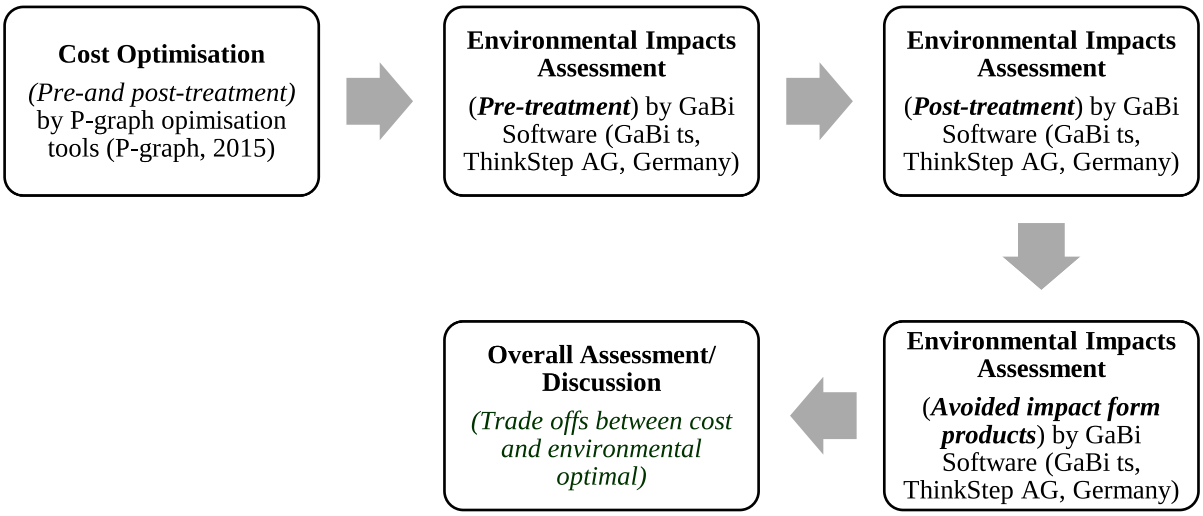


Figure 5.11: Flow structure in identifying the optimal pre-treatment and post-treatment pathway

In this study, LW is assumed to have the potential biogas yield of 400 m^3 biogas/t as according to NNFCC (2017). The amount of biogas without pre-treatment is 50 % of the potential biogas yield. This assumption is based on Azman et al. (2015). The sustainable options in term of economics were identified using the P-graph approach, studio version: 5.2.1.4 (P-graph studio, 2015). P-graph is a combinatorial optimisation framework aimed at optimising process networks (Friedler et al., 1992) and has been recently used to propose the utilising network of municipal solid waste (Walmsley et al., 2017).

The environmental impacts which include global warming potential (GWP), human toxicity, ozone depletion potential (ODP), particulate matter (PM), photochemical oxidant creation (POCP), acidification (AP) and eutrophication potential (EP) were evaluated by using GaBi Software ts version 2017 (Thinkstep AG, 2017). Even when environmental footprints are offering better quantification and have been increasingly used (Čuček et al., 2014), the environmental impacts are selected due to the well-established database implemented in GaBi Software. The selected impact categories are important, and it has been implemented in different life cycle studies such as by Yasar et al. (2017). The recommended International Reference Life Cycle Data System (ILCD) method, as in the GaBi Software is applied in the study. The selected database from GaBi is the case of the EU. For example, the electric grid mix is based on EU28 where nuclear (27.1 %) has the highest share, followed by hard coal (16.1 %), natural gas (15.7 %), heavy fuel (12.4 %) and lignite (10.1 %) and others.

5.2.3 Case Study

In this study, a P-graph framework is developed to assess eight different types of pre-treatment and post-treatment. The pre-treatment alternatives include grinding (P1), steam explosion (P2), water vapour (P3), CaO (P4), NaOH (P5), H_2SO_4 (P6), enzyme (P7) and microbial consortium (P8) - See Table 5.10. The post-treatments consist of post-treatment for fuel cell (FC), combined heat and power (CHP), biofuel (BF) and biomethane (H_2S removal + pressure water scrubbing (HSR PWS), H_2S removal + organic physical scrubbing (HSR OPS), H_2S removal + amine scrubbing (HSR AS), H_2S removal + pressure swing adsorption (HSR PSA), H_2S removal + membrane separation (HSR MS) - see Table 5.11.

Table 5.10 and 5.11 summarised the type and the input data of different pre-treatment and post-treatment applied in this study. The major operating cost of pre-treatment and post-treatment was considered. The comparison is made on the same basis, although some of the costings are not taken into consideration. For example, the operation cost (€/t) of the AD was excluded from all the pathways with the assumption that the AD system is the same. The capital and maintenance costs are excluded in the costing.

Table 5.10: The output and main operating cost of different pre-treatment for AD

Pre-treatment	Output[c] (m^3 biogas/t)	Reference	Main Operating Cost[a,d] (€/t)
1. No treatment (P0)	200	Azman et al. (2015)	-
2. Grinding (P1)	220	Mönch-Tegeder et al. (2014)	1.498
3. Steam explosion (P2)	232	Bauer et al. (2014)	1
4. Water vapour (P3)	208.6	Li et al. (2012)	0.12
5. CaO (P4)	318	Bruni et al. (2010)	10.56
6. NaOH (P5)	256	Sambusiti et al. (2012)	35.2
7. H_2SO_4 (P6)	231	Taherdanak et al. (2016)	2.64
8. Enzyme (P7)	255.8	Ziemiński and Kowalska-Wentel (2015)	11
9. Microbial consortium (P8)	393.26	Zhang et al. (2011)	840[b]

[a]Only the main operating cost of the process, e.g. the electric/heat, the chemical cost for chemical treatment, the cost of the enzyme for biological treatment etc. were included. [b]Small scale experimental study, not necessarily reflect the large-scale implementation. [c]Calculated based on the reported enhancement of biogas. [d]Price of consumables. CaO = 176 €/t, H_2SO_4 = 264 €/t, Enzyme = 1.1 €/t, NaOH = 352 €/t, Peptone = 0.126 €/g.

Table 5.11: The output and main operating cost of different post-treatment for AD

Post-treatment	Output (kWh/m^3 biogas)[b]	Reference	Main Operating Cost[a,c] (€/t)
• Biogas			
1. H_2S removal + pressure water scrubbing (HSR PWS)	9.500	Leme and Seabra (2017)	0.252
2. H_2S removal + organic physical scrubbing (HSR OPS)	9.409	Leme and Seabra (2017)	0.026
3. H_2S removal + amine scrubbing (HSR AS)	9.895	Leme and Seabra (2017)	0.076
4. H_2S removal + pressure swing adsorption (HSR PSA)	8.924	Leme and Seabra (2017)	0.036
5. H_2S removal + membrane separation (HSR MS)	9.752	Leme and Seabra (2017)	0.040

6.	Biofuel (BF)	6.370	Larsson et al. (2015)	0.189
7.	Combined heat and power (CHP)	2.27 (Heat), 1.81 (Electricity)	Wu et al. (2016)	0.015
8.	Fuel cell (FC)	2.31 (Heat), 1.54 (Electricity)	Wu et al. (2016)	0.021
9.	No post-treatment (NA)	0.6 m^3 of CH_4/ m^3	-	-
•	Digestate			
1.	Sterilisation and composting	0.5 t compost/t digestate	Pöschl et al. (2010)	1.26
2.	No-treatment	0.9 t digestate/t feedstock	-	-

[a]Only the main operating cost of the process, e.g. the electric/heat, water consumption for water scrubbing, the chemical cost for chemical treatment, the cost of the enzyme for biological treatment etc were included. [b]Unit of the output, unless stated. [c]Water = 0.54 €/m^3.

Although some cost items have not been considered in this case, the P-graph framework offers the room to include the information for optimisation when the data is available. Figure 5.12 shows the P-graph interface for “Operating unit”. In this study, “Operating unit” refers to the pre- and post-treatment process, see the highlighted rectangular boxes by red lines in Figure 5.13. The model/superstructure representing the AD process of LW to be applied in this study is illustrated in Figure 5.13. The potential product materials of the AD process are heat, electricity, biofuel, digestate and compost. It shows the all possible connections of different pre-treatment and post-treatment alternatives.

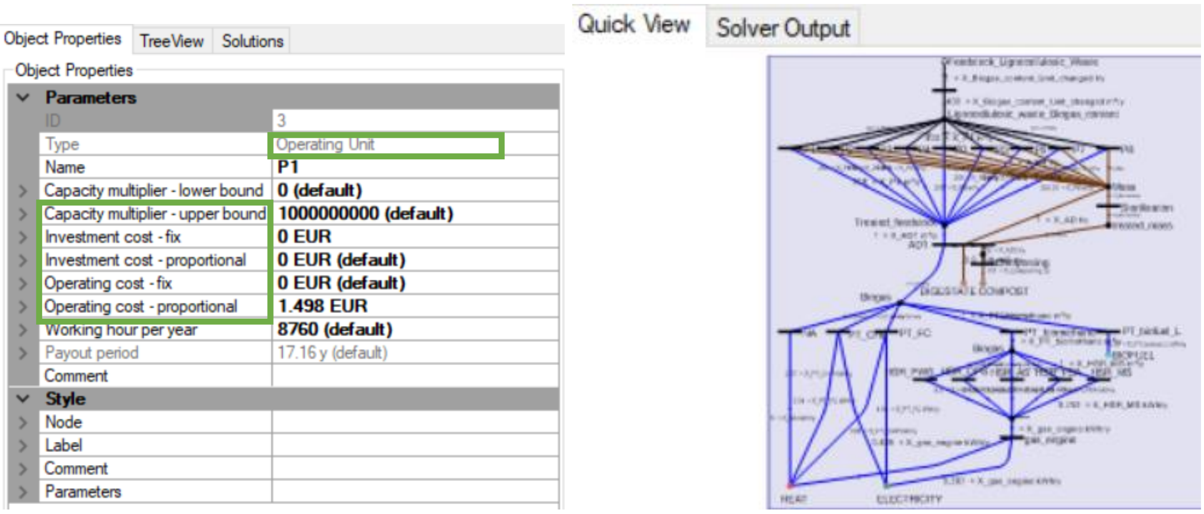


Figure 5.12: P-graph interface. The data input column of P1 (Operating Unit)

Table 5.12 shows the important conversion factors and assumptions made. The input of LW is assumed to be 100 t/y in applying the P-graph optimisation. The reported value in the results and discussion did not reflect the actual profit of the respective AD pathways. It serves as an indicator for the cost optimised pre-treatment and post-treatment pathway, where a higher value reflects higher feasibility. The cost-optimal and near-optimal solutions identified by P-graph were further discussed by considering the environmental impacts. Sensitivity analysis is conducted to curtail the uncertainty of the input data (fluctuations, inflation, range of cost data) and enhance the robustness of the identified result. The effect of changing the cost of pre-treatments and post-treatments (by applying 5%, 10%, 15% and 20% reduction and increment) on the optimal solution and the objective function values (maximum profit) are identified.

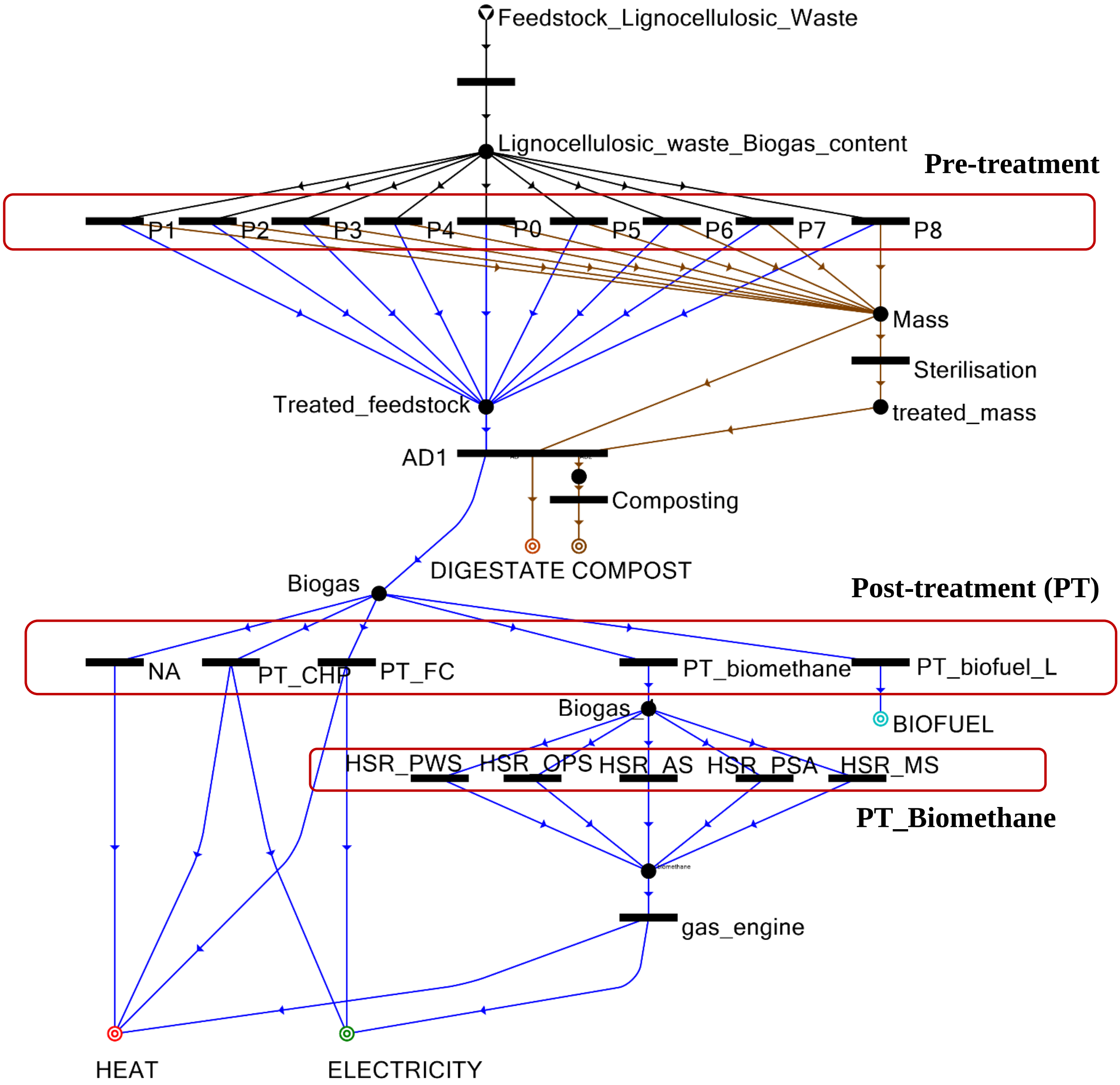


Figure 5.13: P-graph representation of the assessed AD study

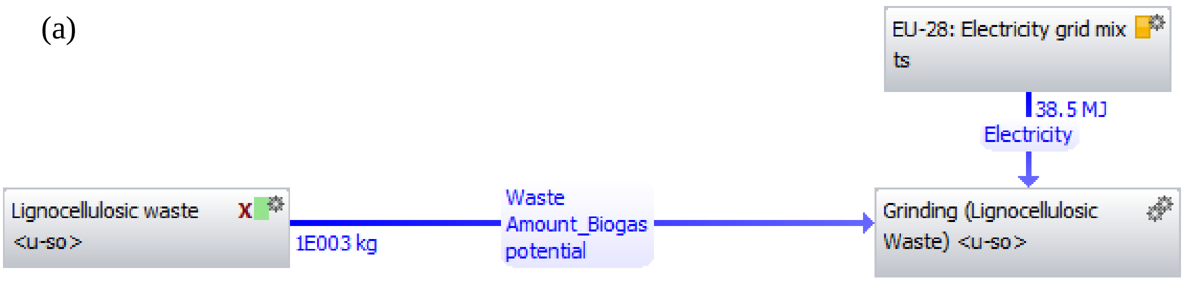
Table 5.12: The assumptions and conversion factors

Assumptions/conversion factors	Reference
The potential biogas yield of lignocellulosic feedstock = 400 m^3/t	NNFCC (2017)
Electricity = 0.14 €/kWh	Wu et al. (2016)
Heat energy = 0.04 €/kWh	Wu et al. (2016)
Biofuel = 0.119 €/kWh	Larsson et al. (2015)
Compost = 3.81 €/t	Meyer-Kohlstock et al. (2015)
Digestate = 1.81 €/t	De Clercq et al. (2017)
The thermal and electrical efficiency of gas engine = 48.5 % and 38.7 %	Jenbacher Type 2
1 m^3 CH_4 = 10 kWh	Charles (2009)

Conversion rate, July 2017: 1 BRL (Brazilian Real equals) = 0.27 €; 1 USD (US Dollar) = 0.88 €; 1 RMB (Renminbi/Chinese Yuan) = 0.13 € (GoogleFinance, 2017).

Figure 5.14(a) - (f) shows the scopes of study in identifying the environmental impacts of the pre-treatments. Biological pre-treatment (enzyme and microbial consortium) is excluded due to the lack of information about the environmental impact to produce the enzyme and microbial consortium. The impacts are assumed to be minimal as biological pre-treatment is known to be environmentally friendlier than physical and chemical treatments.

(a)



(b)

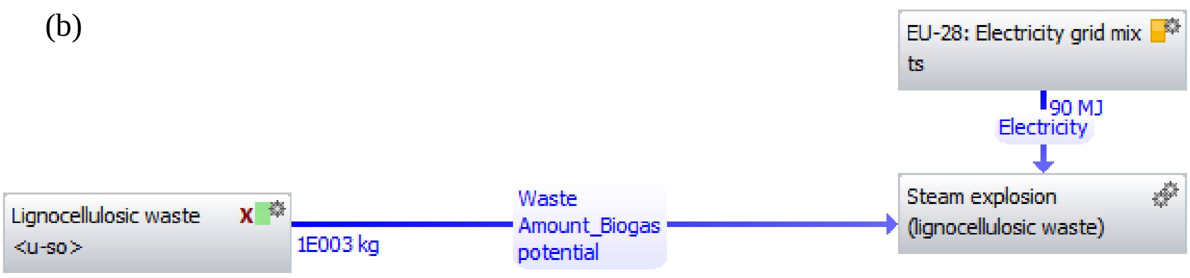
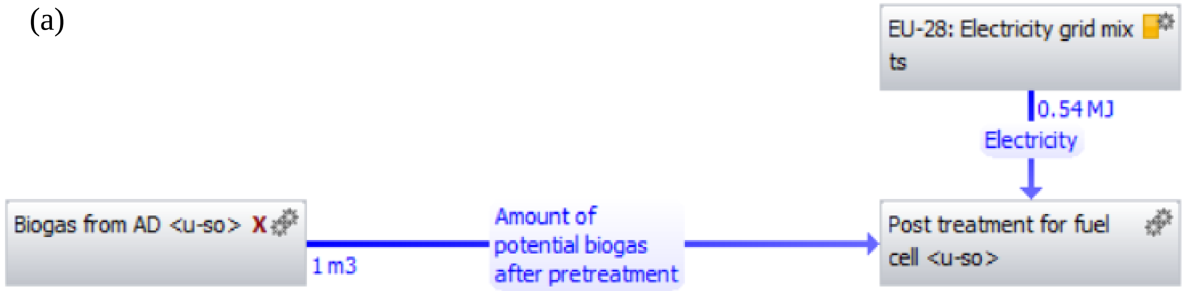


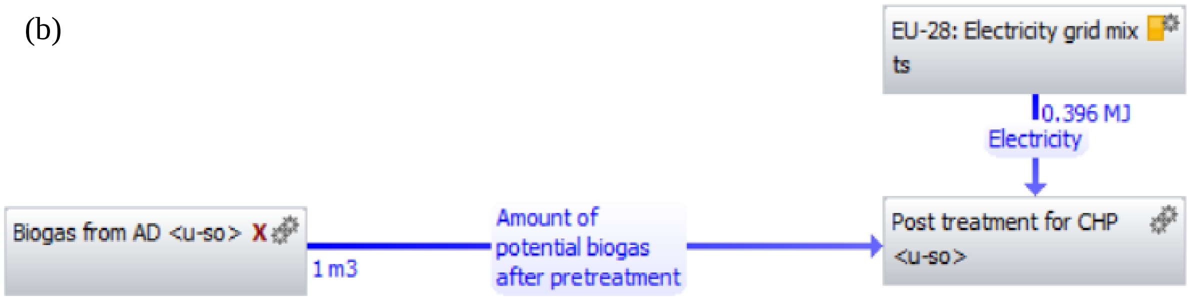
Figure 5.14: The assessed components in identifying the environmental impacts of pre-treatments a) grinding (P1), b) steam explosion (P2), c) water vapour (P3), d) CaO (P4), e) NaOH (P5), f) H_2SO_4 (P6). The presented value is based on Table 31 and 32.

Figure 5.15 shows the included components in identifying the environmental impact of the post-treatments of biogas. Figure 5.14 and 5.15 are constructed based on the required input, as stated in Table 5.10 and 5.11. The environmental impacts of the pre-treatment and post-treatment were identified by referring to the required input material for the processes, e.g. electricity, chemicals, water. The reported values are per t (0.001 kg/t) of LW for pre-treatment and per m^3 of biogas for post-treatment.

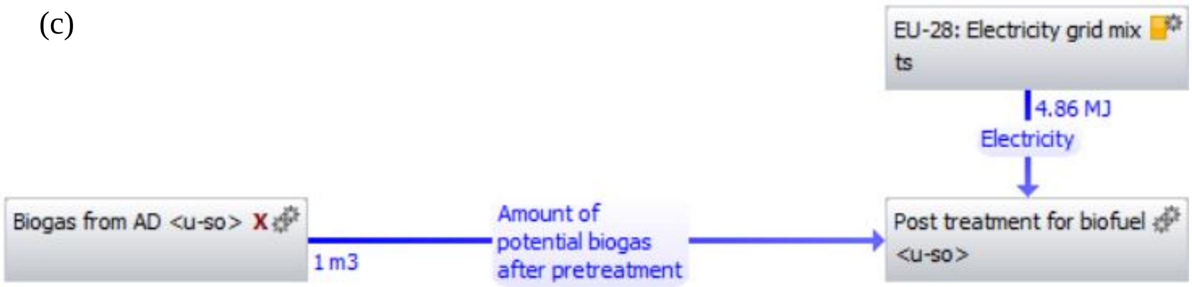
(a)



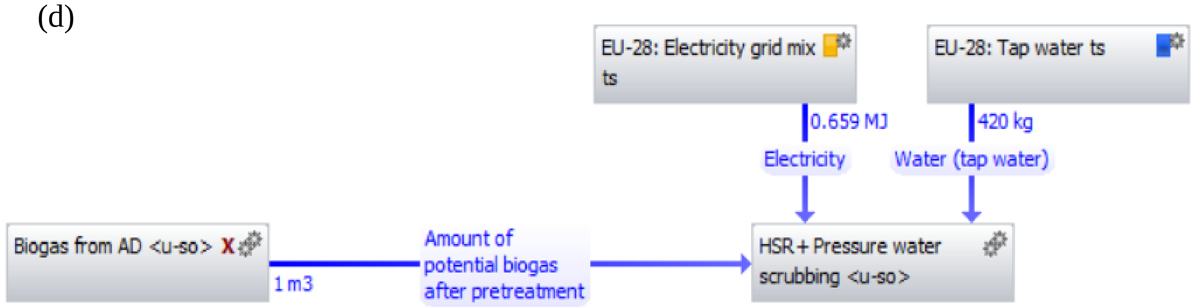
(b)



(c)



(d)



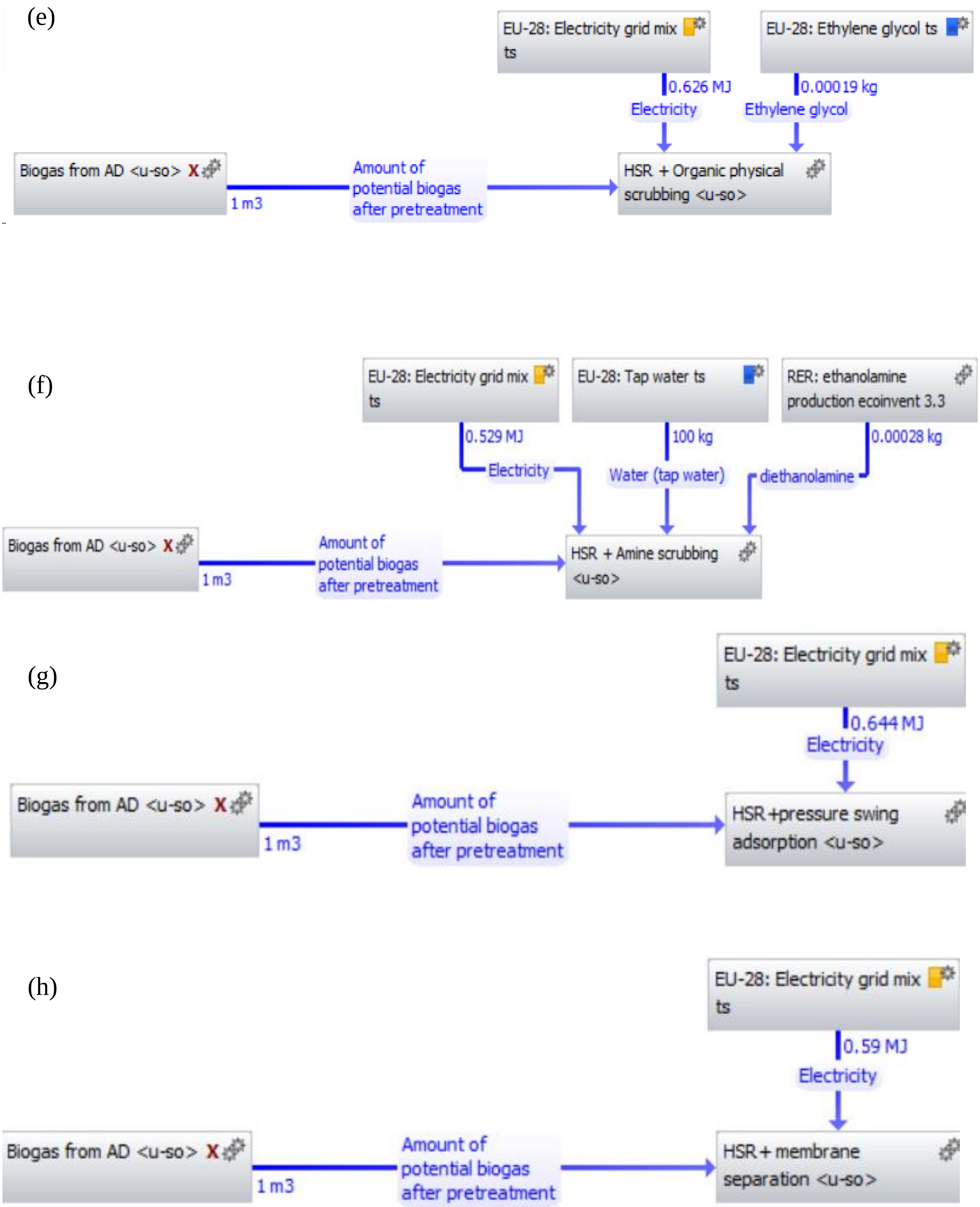


Figure 5.15: The assessed components in identifying the environmental impacts of post-treatments (a) Fuel cell (FC), (b) Combined heat and power (CHP), (c) Biofuel (BF), (d) H_2S removal + pressure water scrubbing (HSR PWS), (e) H_2S removal + organic physical scrubbing (HSR OPS), (f) H_2S removal + amine scrubbing (HSR AS), (g) H_2S removal + pressure swing adsorption (HSR PSA) (h) H_2S removal + membrane separation (HSR MS), constructed by GaBi Software.

The gross compensated environmental impacts were identified by considering the avoided impacts from the conventional method of producing the biogas products (electricity, gasoline/fuel and heat), based on Eq(5.2)

$$Gross\ Avoided\ Impacts = Environmental\ Impacts\ Factors\ x\ Quantity\ of\ Products \quad (5.2)$$

The gross avoided impacts from the generation of electricity, gasoline and heat are reported as unit/m^3 of biogas, where the unit is listed in Table 5.13. The accessed environmental impacts include GWP, ODP, Human toxicity, PM, POCP, AP, EP, where the impact factors are generated by GaBi software (GaBi ts, AG ThinkStep, Germany), see Table 5.13. The quantity of products (output) of each post-treatment approaches is listed in Table 5.11. The overall environmental impacts of post-treatments (cost-optimal and near-optimal alternatives) were estimated by Eq(5.3), where the environmental impacts in performing the post-treatment process were divided by the gross avoided impacts. A smaller value was interpreted as a more environmental friendlier option. It did not reflect the actual environmental impacts as this study only considered the impact of the main operation as specified in Table 5.10 and 5.11. Transportation etc. is excluded. The calculation is based on 1 m^3 of biogas from the post-treatment.

$$Overall\ Impacts = Environmental\ impacts\ in\ performing\ post\ treatment - gross\ avoided\ impacts \quad (5.3)$$

Table 5.13: Environmental impacts per unit of electricity (electric grid mix), gasoline and heat, specified for the case of EU-28 by GaBi database (Thinkstep AG, 2017)

Environmental impacts	Units used	Environmental impacts factors		
		Electricity (unit[a]/kWh)	Gasoline (unit[a]/m^3)	Heat (unit[a]/kWh)
GWP (excluded biogenic CO_2)	kg CO_{2eq}	0.444	0.579	0.255
ODP	kg $R11_{eq}$	1.97×10^{-11}	1.67×10^{-12}	3.67×10^{-13}
Human Toxicity (cancer)	CTUh	3.97×10^{-10}	1.75×10^{-8}	3.37×10^{-11}
PM	$PM2.5_{eq}$	7.48×10^{-5}	1.63×10^{-4}	7.28×10^{-6}
POCP	kg $NMVOC_{eq}$	7.32×10^{-4}	1.68×10^{-4}	1.44×10^{-4}
AP	mole of H^+_{eq}	1.41×10^{-3}	2.60×10^{-3}	1.44×10^{-4}
EP	mole of N_{eq}	2.79×10^{-3}	5.03×10^{-3}	3.52×10^{-4}

CTUh = Comparative Toxic Unit for human. NMVOC = Non-methane volatile organic compound. R11 = trichlorofluoromethane. Eq = equivalent. [a]Refer to the unit column for the respective unit of different environmental impacts categories

5.2.4 Results and Discussion

Figure 5.14 shows the optimal pathway by P-graph according to the cost assessment. The CaO pre-treatment (P4) and H_2S removal + membrane separation (HSR MS) post-treatment are identified as the best option, with heat, electricity and digestate as the product materials. The alkali CaO (P4) pre-treatment requires a higher operating cost than the physical approaches such as grinding (P1) and steam explosion (P2). However, it is offering a higher enhancement of the yield of biogas (59 %, from 200 m^3/t to 310 m^3/t), see Table 5.11.

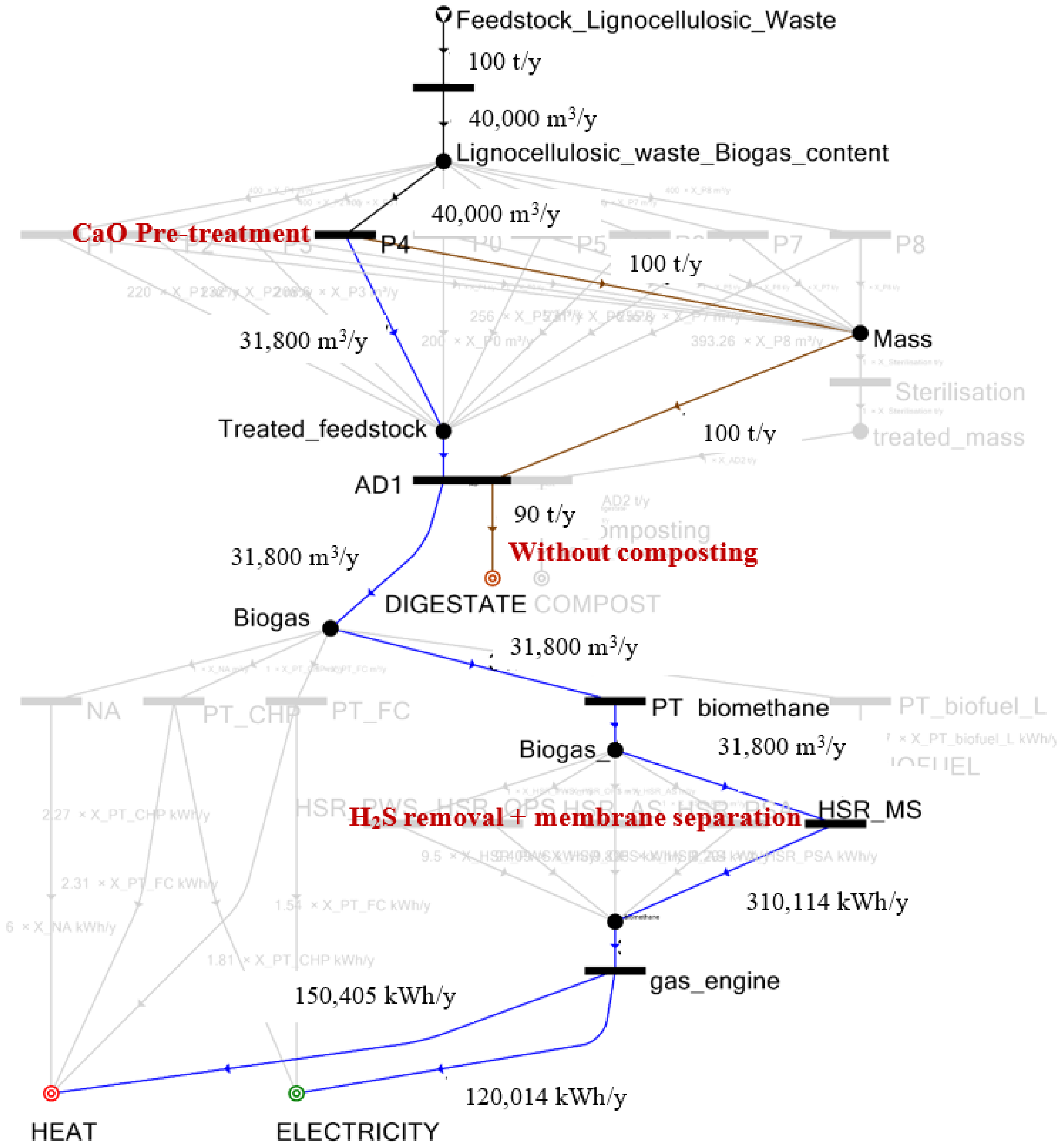


Figure 5.14: Optimum solution for minimum cost with P-graph representation

The reported retention time for CaO treatment is 10 d. This proposes there is a need for more holding vessel and higher investment cost for the same capacity to handle the same amount of LW/d. This suggests the CaO (P4) option could be less feasible if the investment cost is limited. The investment cost is not considered in this study. The environment footprints need to be further evaluated as that is the major disadvantage of chemical treatments. HSR MS post-treatment was identified as the most suitable pathway in the economic perspective. Although the main operating cost of HSR MS is higher than HSR PSA and HSR OPS, the value of products (heat and electricity) are higher, where the estimated profit is higher (20,653.0 €/y, see Table 5.14). The upgraded treatment enhanced the quality/purity of methane in the biogas as well as the energy value and selling price.

Table 5.14: Top 5 feasible (optimal/near-optimal) structures identified by P-graph

Feasible structure	Value (€/y) *
P4, HSR MS, without composting (as shown in Figure 5.14)	20,653.0
P4, HSR MS, with composting	20,523.0
P4, HSR OPS, without composting	20,307.1
P4, HSR OPS, with composting	20,189.6
P4, HSR AS, without composting	19,856.8

*Indicator for the optimised pathway, where a higher value reflects higher feasibility. It did not reflect the actual profit. The calculation is based on 100 t/y of LW.

This study did not limit itself to the generation of a single optimal solution. The other near-optimised solutions by P-graph are summarised in Table 5.14. It should be noted that the presented value in Table 5.14 did not reflect the actual profit. The estimation is based on the main consumables and operating cost. It is used as the indicator of the optimal pathway, where a higher value reflects higher economic feasibility. Based on Table 5.14, there are no changes in the pre-treatment alternative. P4 remains as the suggested options. The near-optimal post-treatments for biogas treatment are HSR OPS (20,307.1 €/y) and HSR AS (19,856.8 €/y). The digestate management did not have a significant role in the profit (see Table 5.14). According to the analysis, composting of digestate is comparatively less feasible than no treatment (without composting). The selling price of compost (3.81 €/t) is higher than the digestate (1.81 €/t), but the operating cost is significant, yet the product yield is 50 % lesser than the digestate (see Table 5.12). This result could be subjected to the policy and the pricing in different countries. Digestate cannot be applied directly to the soil in some countries. The digestate value could be lower than the value stated in this study or even negative if ended in the landfill due to tipping fees and transportation cost etc. The suggested feasible structures/pathways in Table 5.14 are solely by considering the economic factors. The environmental and other real-world constraints should also take into consideration towards a sustainable treatment pathway.

The environmental impacts of different pre-treatments were assessed, as shown in Figure 5.15. The environmental impacts of CaO pre-treatment (P4), which represents the low-cost approach, is presented in Table 5.15. The environmental impacts are not as low as the biological treatment (P7 and P8) and water vapour pre-treatment (P3). However, it is an option with higher cost feasibility. NaOH pre-treatment (P5) has the worst environmental performance in GWP, ODP, human toxicity, POCP and EP. H_2SO_4 pre-treatment (P6) has the worst environmental performance in AP and PM. No consistent trend is conclusive to decide which is the environmental friendliest approach as its impacts on the environment in a different way. In general, P7, P8, P3 have relatively low environmental impacts. P1, P2 and P4 are in the medium range. P5 and P6 are in the higher range.

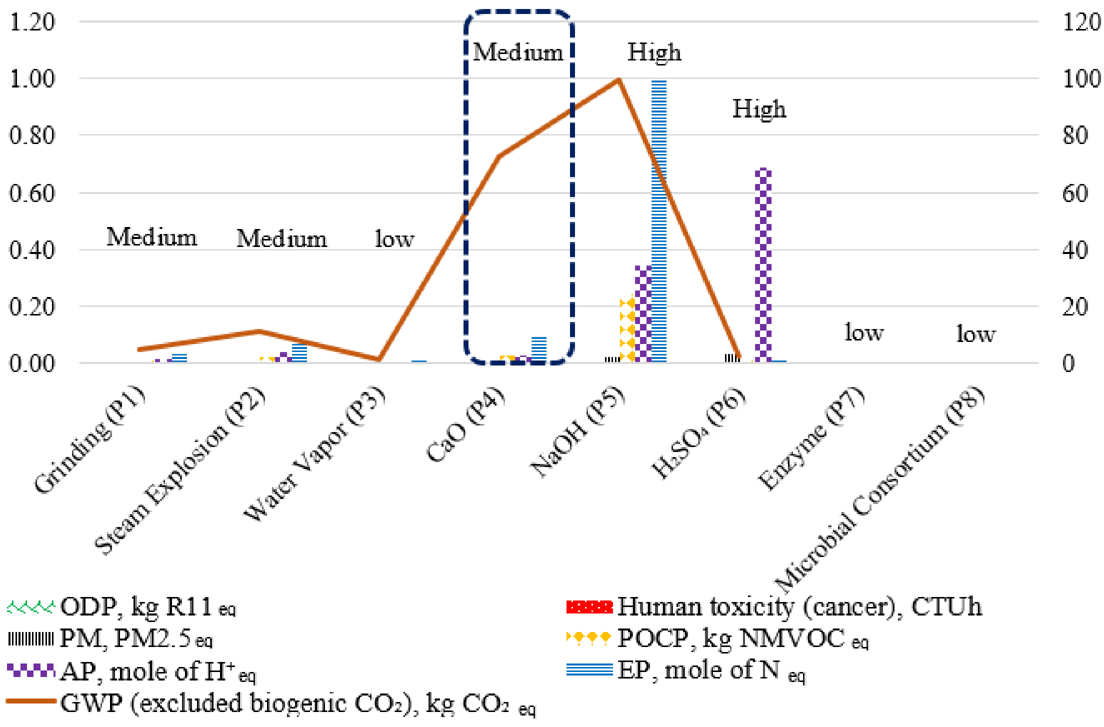


Figure 5.15: The environmental impacts of different pre-treatment options for LW. Blue dotted box highlighting the cost-optimal solution. Right scale (secondary axis) is for global warming potential. The units are as stated in the legend per t of LW.

The environmental impacts of different post-treatments are shown in Figure 5.16a and b. Post-treatment of CHP shows the best environmental performance in all the assessed environmental impacts. HSR PWS has the highest impact (worst environmental performance) in term of human toxicity (1.39 x 10^{-9} CTUh/ t of LW), PM (5.32 x 10^{-4} $PM2.5_{eq}$/ t of LW), POCP (4.49 x 10^{-4} kg NMVOC $_{eq}$/t LW), AP (6.38 x 10^{-4} mole of H^{+} $_{eq}$/ t of LW) and EP (1.74 x 10^{-3} mole of N $_{eq}$/t of LW). HSR MS, HSR AS and HSR OPS (see Figure 5.16a and b, dotted boxes) are the cost-optimal and near-optimal solutions. However, by referring to the environmental impacts, HSR AS has the worst performance in term of GWP (1.01 x 10^{-1} kg CO_2 $_{eq}$/t of LW) and ODP (4.47 x 10^{-11} kg R11 $_{eq}$/t of LW). This suggests HSR OPS and HSR MS are the post-treatment which are comparatively feasible in term of both cost and environmental impacts.

Table 5.15: The environmental impacts of the identified cost-optimal solution (CaO pre-treatment, P4)

	CaO pre-treatment (P4)	The worst
GWP (excluded biogenic CO_2), kg $CO_{2\ eq}$	72.6	99.0 (P5)
ODP, kg R11eq	4.58 x 10^{-11}	3.08 x 10^{-9} (P5)
Human toxicity (cancer), CTUh	6.57 x 10^{-8}	1.36 x 10^{-7}(P5)
PM, $PM_{2.5eq}$	1.76 x 10^{-3}	3.29 x 10^{-2} (P6)
POCP, kg $NMVOC_{eq}$	2.55 x 10^{-2}	2.46 x 10^{-1} (P5)
AP, mole of $H^{+}_{\ eq}$	2.50 x 10^{-2}	6.88 x 10^{-1} (P6)
EP, mole of N_{eq}	9.31 x 10^{-2}	1 (P5)

The avoided environmental impacts from the AD of LW by applying the different post-treatments are tabulated in Table 5.16. In general, post-treatment for BF offers the least unburdening effect (avoided environmental impacts), see grey shade (italic and bold). The biofuel produces through the post-treatment offers a high avoided impact in term of human toxicity (1.11 x 10^{-8} CTUh); however, not in the other assessed impact categories. This suggests the utilisation of biogas as heat and electricity provides better-avoided impacts in overall than biofuel utilisation.

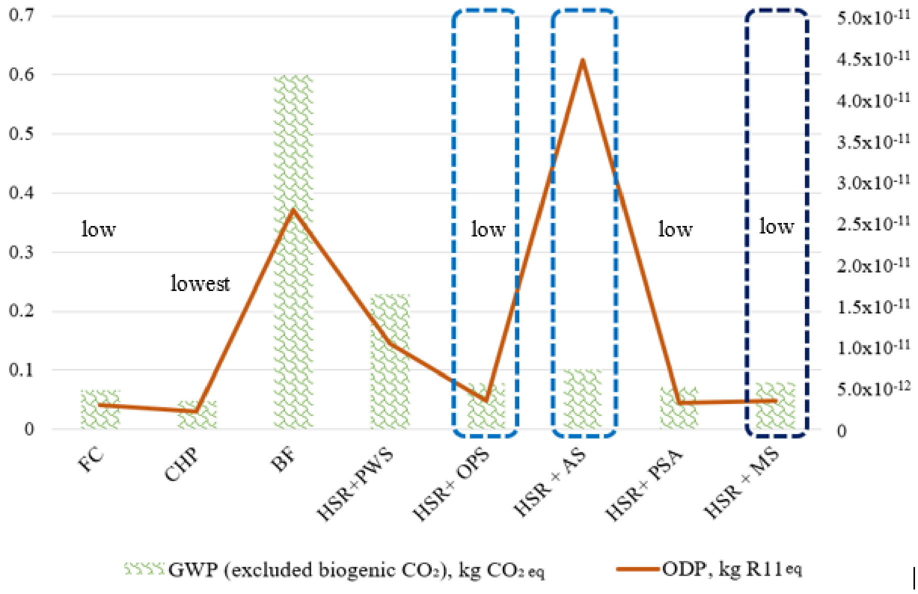


Figure 5.16a: The environmental impacts (GWP and ODP) of different post-treatment options for LW. Dark dotted blue box highlighting the cost-optimal solution and light blue showing the near-optimal solutions. Right scale (secondary axis) is for ODP. The units are as stated in the legend per m^3 of biogas.

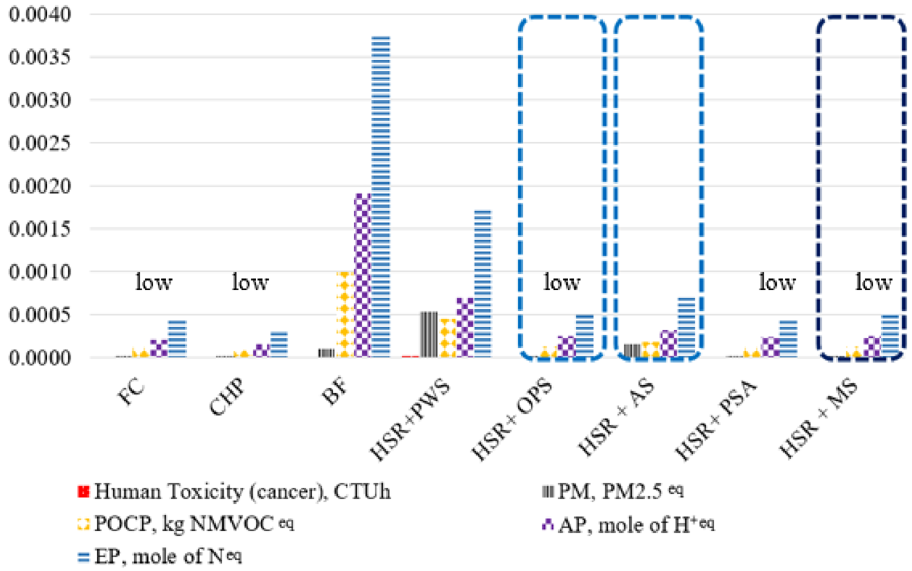


Figure 5.16b: The other environmental impacts of different post-treatment options for LW. The broken line box in dark blue colour is highlighting the cost-optimal solution and light blue showing the near-optimal solutions. The units are as stated in the legend per m^3 of biogas.

By assessing the highlighted (See Table 5.16, dotted blue boxes) cost-optimal and near-optimal solutions (HSR MS, HSR OPS, HSR AS), HSR AS is having a better score in term of avoided environmental impacts. However, HSR MS and HSR OPS are more competitive in cost (higher profit) and environmental impacts (lower impacts), suggesting greater feasibility for implementation. Table 5.17 shows the overall environmental impacts of different post-treatments. HSR MS and HSR AS are having better overall environmental impacts performances than HSR OPS. HSR MS has the lowest OD, Human Toxicity, and PM. HSR AS has the lowest GWP, POCP, AP, and EP. This study identifies a wider range of options. This enables better decision making based on the constraints and environmental concern at a place.

Table 5.16: The avoided environmental impacts from the AD of LW by applying different post-treatments

	FC	CHP	BF	HSR PWS	HSR OPS	HSR AS	HSR PSA	HSR MS
GWP (excluded biogenic CO_2), kg CO_{2eq}	1.42	1.38	***0.37***	2.81	2.78	**2.92**	2.64	2.81
ODP, kg $R11_{eq}$	4.61 x10^{-11}	3.65 x10^{-11}	***1.06 x10^{-12}***	7.41 x10^{-11}	7.34 x10^{-11}	**7.72 x10^{-11}**	6.96 x10^{-11}	7.60 x10^{-11}
Human toxicity (cancer), CTUh	9.64 x10^{-10}	***7.91 x10^{-10}***	**1.11 x10^{-8}**	1.61 x10^{-9}	1.59 x10^{-9}	1.67 x10^{-9}	1.51 x10^{-9}	1.64 x10^{-9}
PM, $PM_{2.5eq}$	1.84 x10^{-4}	1.52 x10^{-4}	***1.04 x10^{-4}***	3.09 x10^{-4}	3.06 x10^{-4}	**3.21 x10^{-4}**	2.90 x10^{-4}	3.15 x10^{-4}
POCP, kg $NMVOC_{eq}$	1.91 x10^{-3}	1.65 x10^{-3}	***1.07 x10^{-3}***	3.35 x10^{-3}	3.32 x10^{-3}	**3.49 x10^{-3}**	3.15 x10^{-3}	3.40 x10^{-3}
AP, mole of H^+_{eq}	3.48 x10^{-3}	2.88 x10^{-3}	***1.66 x10^{-3}***	5.85 x10^{-3}	5.79 x10^{-3}	6.09 x10^{-3}	5.49 x10^{-3}	**5.96 x10^{-3}**
EP, mole of N_{eq}	6.99 x10^{-3}	5.85 x10^{-3}	***3.20 x10^{-3}***	1.19 x 10^{-2}	1.18 x10^{-2}	**1.24 x10^{-2}**	1.12 x10^{-2}	1.21 x10^{-2}

The broken line box in dark blue colour is highlighting the cost-optimal solution and light blue showing the near-optimal solutions. Grey shade (italic and bold) represents the least feasible option when considering the avoided impacts from the products, where the value of avoided impacts is low. Green shade (bold) represents the most feasible option when considering the avoided impacts from the products, where the value of avoided impacts is high.

Table 5.17: Overall environmental impacts (Environmental impacts of post-treatments – Gross avoided impacts from the product)

	HSR OPS	HSR AS	HSR MS
GWP (excluded biogenic CO_2), kg CO_{2eq}	-2.70	**-2.82**	-2.73
ODP, kg $R11_{eq}$	-7.00 x 10^{-11}	-3.25 x 10^{-11}	**-7.24 x 10^{-11}**
Human Toxicity (cancer), CTUh	-1.53 x 10^{-9}	-1.27 x 10^{-9}	**-1.58 x 10^{-9}**
PM, $PM2.5_{eq}$	-2.93 x 10^{-4}	-1.72 x 10^{-4}	**-3.01 x 10^{-4}**
POCP, kg $NMVOC_{eq}$	-3.20 x 10^{-3}	**-3.31 x 10^{-3}**	-3.27 x 10^{-3}
AP, mole of H^{+}_{eq}	-5.54 x 10^{-3}	**-5.77 x 10^{-3}**	-5.71 x 10^{-3}
EP, mole of N_{eq}	-1.13 x 10^{-2}	**-1.17 x 10^{-2}**	-1.16 x 10^{-2}

A smaller value (more negative) reflects better environmental performance. It did not reflect the actual environmental impacts as this study only considered the impact of the main operation. Transportation etc. is excluded. The calculation is based on 1 m^3 of biogas from the post-treatment. Green shade (bold) represents the most feasible option of the respective environmental impacts' categories.

5.2.4.1 Sensitivity Analysis and Overall Discussion

Sensitivity analysis has been performed to assess the identified optimal solution (P4 and HSR MS) under a different range of operating cost. Figure 5.17 shows the analysis results. Under most of the changes, P4 + HSR MS remains as the best solution. By referring to Table 5.14, P4 +HSR MS is still a better solution only if the value is less than 20,307.1 €/y. The near cost-optimal solution P4 + HSR OPS (Table 5.14) is a better option when the operating cost of P4 and HSR MS have a more than 10 % increment (See Figure 5.17, bold font in the grey box).

		Operating cost of P4								
	20,653.06	8.448	8.976	9.504	10.032	*10.560*	11.088	11.616	12.144	12.672
Operating cost of HSR MS	0.048	20,609.86	20,557.06	20,504.26	20,451.46	20,398.66	20,345.86	**20,293.06**	**20,240.26**	**20,187.46**
	0.046	20,673.46	20,620.66	20,567.86	20,515.06	20,462.26	20,409.46	20,356.66	**20,303.86**	**20,251.06**
	0.044	20,737.06	20,684.26	20,631.46	20,578.66	20,525.86	20,473.06	20,420.26	20,367.46	20,314.66
	0.042	20,800.66	20,747.86	20,695.06	20,642.26	20,589.46	20,536.66	20,483.86	20,431.06	20,378.26
	0.040	20,864.26	20,811.46	20,758.66	20,705.86	*20,653.06*	20,600.26	20,547.46	20,494.66	20,441.86
	0.038	20,927.86	20,875.06	20,822.26	20,769.46	20,716.66	20,663.86	20,611.06	20,558.26	20,505.46
	0.036	20,991.46	20,938.66	20,885.86	20,833.06	20,780.26	20,727.46	20,674.66	20,621.86	20,569.06
	0.034	21,055.06	21,002.26	20,949.46	20,896.66	20,843.86	20,791.06	20,738.26	20,685.46	20,632.66
	0.032	21,118.66	21,065.86	21,013.06	20,960.26	20,907.46	20,854.66	20,801.86	20,749.06	20,696.26

Figure 5.17: Sensitivity analysis of pre-treatment (P4) and post-treatment (HSR MS) cost. Value in Italic font and in the blue box represents the identified value of the optimal solution, in this study.

The best combination from the perspective of environment impacts is biological treatments + CHP. The biological (P7- Enzyme, P8- Microbial Consortium) and physical (P1- Grinding, P2- Steam Explosion, P3- Water Vapour) pre-treatments alternatives have lower environmental impacts than chemical pre-treatments (P4- CaO, P5- NaOH, P6- H_2SO_4) however they are not part of the near cost-optimal solutions. CHP is the post-treatment with the lowest environmental impacts. Among the near cost-optimal alternatives, post-treatment HSR AS has a better performance in the overall environmental impacts followed by HSR MS and HSR OPS. Although the identified best solutions in term of environmental and cost-optimal are different, there is no significant contradiction. P4 + HRS MS, the suggested cost-optimal solution, has relatively low environmental impacts (see Blue dotted box in Figures 53 and 54) compared to the other options.

5.2.5 Conclusion

This study suggests the sustainable pre-treatment and post-treatments of LW for AD, in term of cost and environmental performances (GWP, ODP, Human toxicity, PM, POCP, AP, EP). CaO pre-treatment (P4), H_2S removal with membrane separation post-treatment (HSR MS) and without the composting of digestate is identified as the cost-optimal pathway for LW (20,653.0 €/y). Each treatment has its limitations. P-graph provides wider rational decision options by considering the near-optimal solutions. The trade-offs between cost and environment performances can be compromised by referring to near-optimal solutions. There is no universal AD solution. Different scenarios (the type of substrate, the scale, product demand, policies) require different solutions.

According to the results from GaBi software, biological pre-treatments (P7 and P8) are having lower environmental impacts than P4. However, they are not within the near cost-optimal solution. NaOH (P5) and H_2SO_4 (P6) pre-treatment have the highest detrimental impact on the environment. In term of post-treatment, the near cost-optimal solutions are H_2S removal with organic physical scrubbing (HSR OPS) and H_2S removal with amine scrubbing (HSR AS). CHP post- treatment which is not within the identified near cost-optimal solution has the lowest burdening impact to the environment. Among the cost-optimal/near-optimal post-treatment alternatives, based on the number of the impact of categories, HSR AS has the lower overall environmental impacts follows by HSR MS and HSR OPS.

The suggested cost-optimal solution (CaO pre-treatment (P4), H_2S removal with membrane separation post-treatment (HSR MS) and without the composting of digestate) has considerately low environmental impacts and cost-effective. The presented study demonstrated the application of P-graph framework and could serve as a guideline in selecting the treatment options. Further assessment is needed in identifying the overall optimal solution by expressing the environmental impacts into the cost and by assigning the appropriate weighting factor. The influence of processing (pre-treatment and post-treatment) or retention time, as well as investment and maintenance costs, can also be studied.

CHAPTER 6

OVERALL CONCLUSION AND RECOMMENDATION FOR FUTURE WORK

Embedding Process Integration into the Circular Economy is essential to ensure that the transition to the circular system is sustainable. Process Integration is a method of taking a holistic approach to process design and optimisation that looks at how a collection of processes or systems are best integrated to ensure the efficient use of energy and achieving a reduction in environmental effects. The novel methodologies proposed in this thesis have emphasised the minimisation of the emission footprints of process design (e.g., waste management and transportation) where the emissions are not solely limited to GHG. Their effectiveness in solving problems was demonstrated through a number of case studies (See Chapters 3-5). The novel methodologies presented have a graphical basis which make them easier for adaption and application as well as having the following other advantageous features (i. they consider both GHG and air pollutants in defining environmental sustainability; ii. they enable integrated regional planning for further emission reduction; iii. they allow comprehensive emission accounting (burdening, unburdening, marginal); iv. they enable the identification of optimal and near-optimal solutions) which offer a wide potential for practical implementation. The specific key insights identified in each of the case studies are summarised as follows.

The breakeven based decision-making (BBDM) tool, which has a similar appearance to a phase diagram, facilitates the rapid selection of transportation modes and biomass utilisation with minimum operating cost and emissions (GHG, SO_2, NO_x and PM). The graphical decision tool can also indicate the next-best solutions when the optimal options are not available. In the transportation case study, an electric train is identified as the cleanest transport mode. However, this result can differ according to the loads, distance, and electricity mix of a particular country. The other key results include: (i) The biodiesel lorry is found to be the best low GHG option for Latvia at R=1 (distance to travel by lorry and train is equivalent), regardless of the load. (ii) In Sweden, the electric lorry is the best transportation mode from both the GHG and Total Environment Burden (TEB) perspective while the electric train is preferable with increasing load. (iii) In the EU-28, biodiesel lorry is the option with the lowest GHG emission, and compressed natural gas when considering the TEB. (iv) Electrification (lorry) generally contributes to a lower TEB in the EU, especially for a country which has a carbon intensity of below average (447 g CO_2eq/kWh). (vi) The bodyweight of transportation has a significant effect on the overall emissions and energy consumption. In the second cases study, BBDM facilitates the selection of biomass utilisation where the highest possible profit and lowest GHG emissions indicate the optimal choice. It is demonstrated by a case study where the biomass (switchgrass and wheat straw) is treated with slow pyrolysis for energy generation or biochar production. Pyrolysis for electricity production is generally a preferable option, especially for countries with high GHG intensity. Biochar application, as a form of carbon emissions sequestration, is suggested at low GHG intensity and becomes preferable when the GHG price is higher than 0.03 USD/kg CO_2eq for switchgrass and higher than 0.01 USD/kg CO_2eq for wheat straw.

The proposed E-WAMPA (Pinch Analysis based methodology) offers an optimisation platform for integrated waste management planning through targeting. It was applied to a municipal solid waste (MSW) case study of the EU to elucidate the application. One of the possible strategies to achieve the 10 % reduction target is demonstrated on the waste treatment transition of Malta (-27.75 kt CO_2eq), Greece (-1,602.71 kt CO_2eq), Cyprus (-178.52 kt CO_2eq) and Romania (-761.16 kt CO_2eq). The proposed methodology has the potential for waste trading planning, offering further emissions reduction by optimising the sharing of resources and facilities. The seasonal availability of the supply and demand market of biomass is one of the challenges for its energy conversion. In the second case study, the production rate, inventory, and supply flow of biomass is identified by integrating Pinch Analysis and mathematical optimisation. The demonstrated case study suggested a fixed production rate of 22,000 GJ/month and adapted to 6,167 GJ/month after the pinch point to meet the fluctuating demand. The required inventory is also suggested. For example, 3,167 GJ of the product (bio-oil) as inventory for Month 4 to meet the following demand, and with 3,764.1 GJ (301 t) of biomass as storage to overcome the supply deficit (fluctuated) in the following month. The mathematical approach optimises the biomass network flow (allocation) at each time interval (month). Emissions and transportation cost, as well as the energy content of the biomass resources, are considered. The proposed extended Pinch Analysis based methodology serves as an effective tool in providing a starting solution dealing with fluctuating supply and demand for further integrated planning.

The P-Graph structure is developed to identify an integrated design of waste management systems in support of a Circular Economy. The case study considers four MSW compositions based on different country income levels. Solving the P-graph model identifies the most suitable treatment approaches, considering the economic balance between the main operating cost, type, yield, quality of products, as well as the GHG emission (externality cost).

The optimal solution for a lower-income country includes a combination of at-source separation, recycling, incineration (heat, electricity), anaerobic digestion (biofuel, digestate) and landfill. It avoids an estimated 411 kg CO_{2eq}/t of processed MSW and achieves a potential profit of 42 € /t of processed MSW. The optimisation generally favours mechanical biological treatment as the country income level rises, which is affected by the composition of the MSW. The relative prices of biofuel, electricity, and heat (>20 %) cause a significant impact on the highest-ranking treatment structure and overall profit. The developed framework produced by P-graph is an effective tool for MSW systems planning. Applying the technique to the pre-and post-treatment assessment of anaerobic digestion, for lignocellulosic waste, the biological and physical pre-treatment alternatives are identified to have lower environmental impacts (global warming potential, human toxicity, ozone depletion potential, particulate matter, photochemical oxidant creation, acidification and eutrophication potential) than chemical pre-treatments. For post-treatment, H_2S removal with amine scrubbing has a better performance in the overall environmental impacts followed by H_2S removal with membrane separation post-treatment and H_2S removal with organic physical scrubbing.

The developed methodologies in this thesis inculcate Process Integration in process design and optimisation. The shared feature is that they consider a system as a whole, which exploits the interactions between different units, to minimise emissions footprints (which includes employing resources effectively) and cost. For example (i) BBDM considers the interactions between air pollutants and GHG (Total Environmental Burden) as well as unburdening and burdening footprints in optimisation. (ii) E-WAMPA, which is an extension of Pinch Analysis (a standard tool of Process Integration), allows for integrated regional waste management planning toward emissions minimisation by complementing each other (e.g. surplus and the deficit of different contributors). (iii) Developed structure by the P-graph technology for an integrated waste treatment system. The performed case studies in this thesis focus on the emissions analyses despite the developed methodologies being capable of including economic concerns. The cost accounting was demonstrated mainly by the operating cost. For future study, comprehensive case studies can be conducted where localised data inputs fed into the proposed methodologies consider the investment cost for a customised and complete solution. A monitoring framework, supported by a combined index (economic, environmental footprints, and material balance), can be developed for a sustainable Circular Economy. Other environmental footprints, e.g. water, can be incorporated into the model.

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APPENDIX

Table S1: The fuel consumption, energy content and price.

Transport mode	Energy[1] MJ/tkm	Fuel Price[2]	Energy Content[3] USD/MJ	Cost USD/tkm
Lorry, light <10 t	0.644	1.29 USD/L	0.0333	0.2264
Lorry, heavy >10 t	0.524	1.29 USD/L	0.0333	0.1099
Diesel Train (container)	0.063	1.29 USD/L	0.0333	0.0123
Electric Train (container)	0.024	86.35 USD/MWh	0.0240	0.0034
Ship (General Cargo)	0.192	805.57 USD/ t	0.0193[4]	0.0042
Ship (Container)	0.030	805.57 USD/ t	0.0193 [4]	0.0042

Conversion factors: 1 Btu=0.00105506 MJ; 1 MWh = 3,600 MJ; 1 gallon= 3.78541 L

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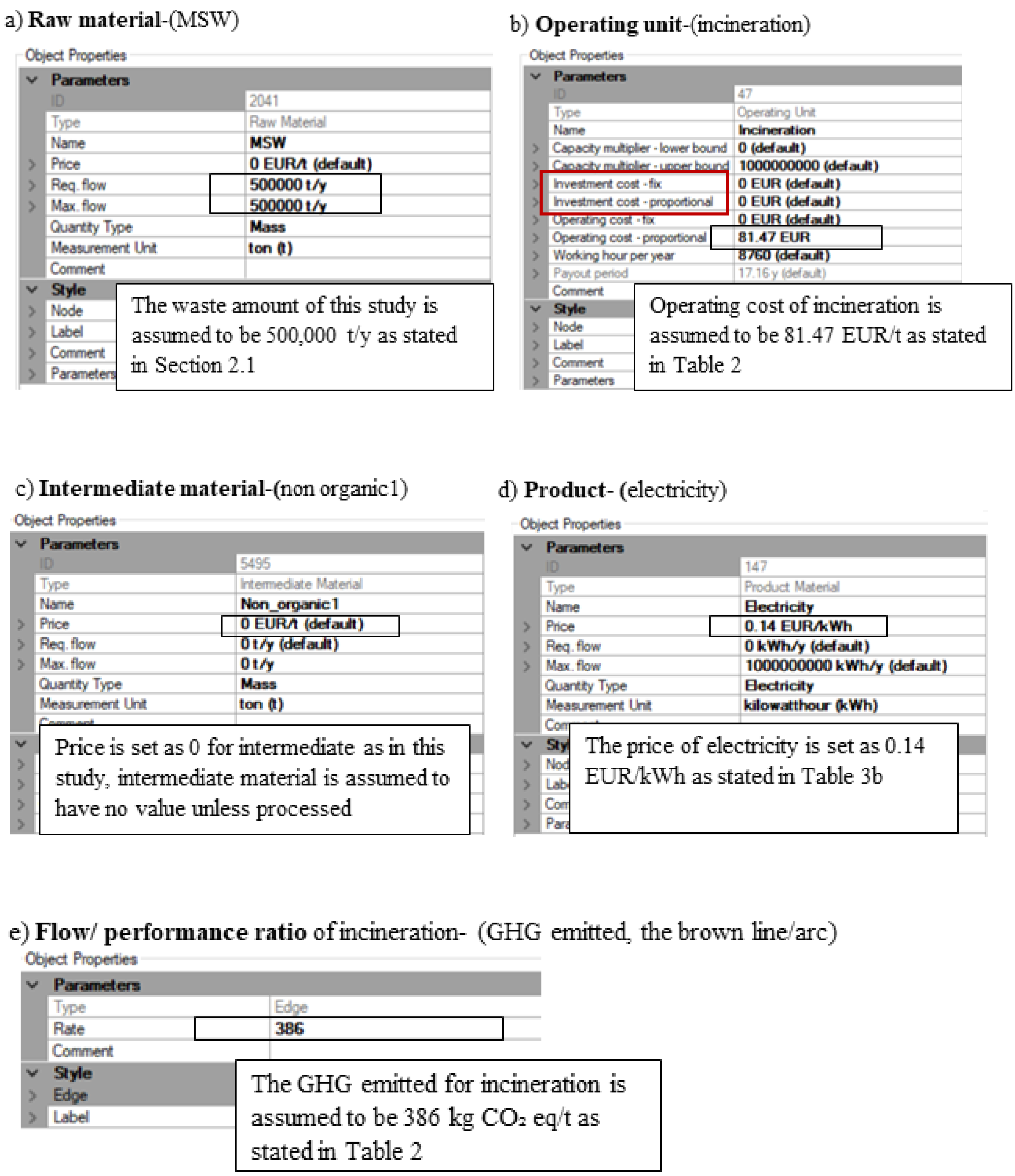

Figure S1: Data input column of five P-graph components and example.

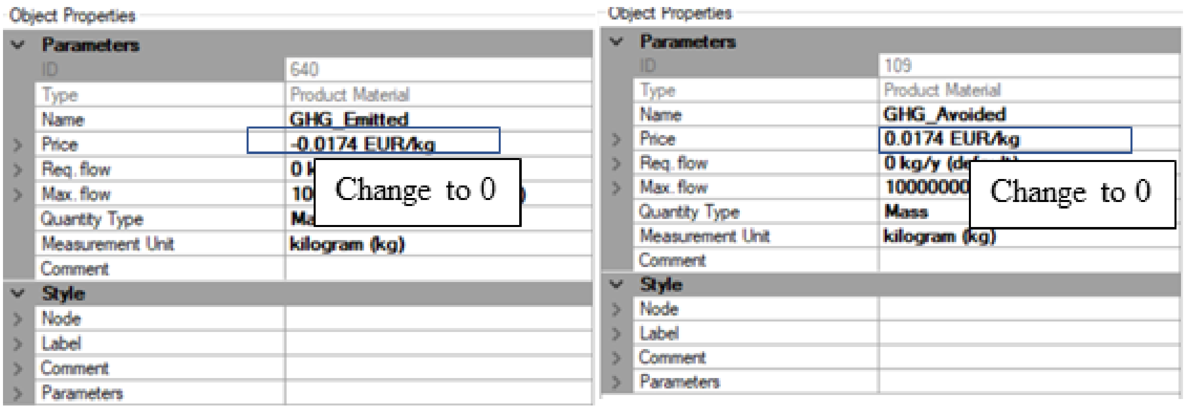

Figure S2: P-graph display of GHG emitted, and GHG avoided for assessing Scope 2-identify the differences in the optimal pathway with and without the consideration of GHG credits.

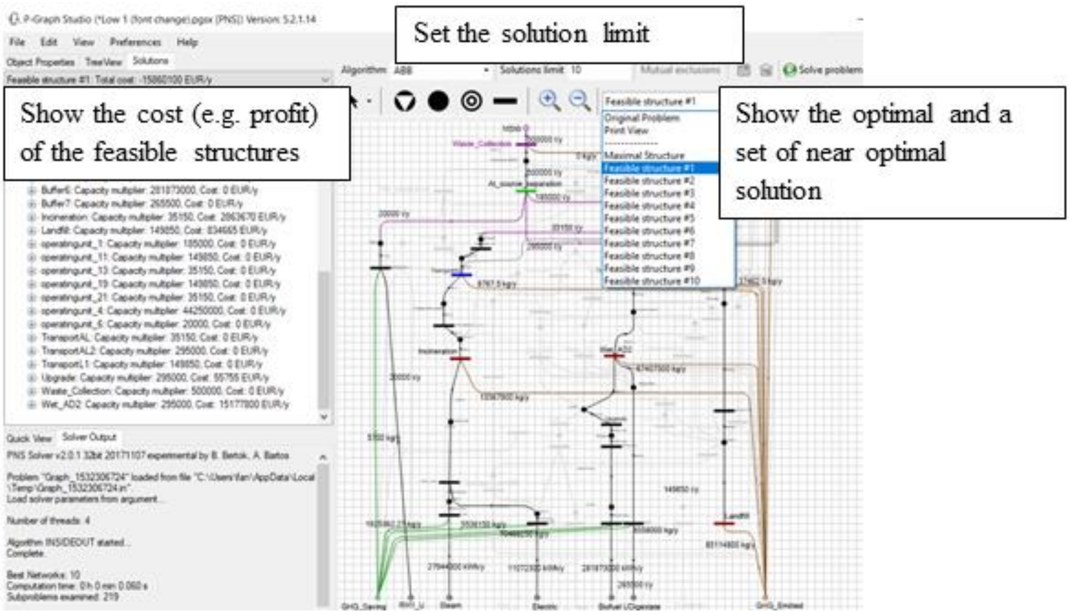

Figure S3: P-graph interface and the results display

Table S2: Conference Presentations

First author and presenter	
1	**Fan YV,** Klemeš JJ, Integrated Framework of Plastic Footprint Toward Regional Circular Economy, 2019 Global Symposium on Waste Plastic- Ecosystem impacts, remediation and waste management. Lexington, Kentucky, US, 19-20 September 2019
2	**Fan YV,** Klemeš JJ, Energy Transition for Sustainable Transportation System: Graphical Approach, International Conference on Energy, Ecology and Environment, Stavanger, Norway, 23-26 July 2019
3	**Fan YV,** Klemeš JJ, Sustainability of Waste Recycling and Recovery Process: EU 28 (27) International Conference on Resource Sustainability- Cities, **Adelaide, Australia,** 1-3 July 2019
4	**Fan YV,** Klemeš JJ, Emission Pinch Analysis for Regional Transportation Planing: Stagewise Approach, 4th International Conference on Smart and Sustainable Technology, **Split and Bol, Croatia**, 28-21 June 2019
5	**Fan YV,** Klemeš JJ, **P-graph Based Waste Treatment Optimisation for Sustainable Recovery**16th IWA World Conference on Anaerobic Digestion, **Delft, Netherland,** 23-27 June 2019.
6	**Fan YV,** Klemeš JJ, Perry S, Lee CT, An emissions analysis for the environmentally sustainable freight transportation modes: Distance and Capacity, 21st Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, **Prague, Czech Republic,** 25 – 29 August 2018.
7	**Fan YV,** Klemeš JJ, Chin HH, Pinch Analysis and Emission Intensity for Waste Management Planning: EU 28, E2S2-CREATE and AIChE Waste Management Conference, CREATE Tower NUS, Singapore, 11-13 March 2019.
8	**Fan YV,** Klemeš, JJ, Walmsley, TG, Perry S, Sustainable Freight Transportation Decision Model in Graphical Representation, Sustainable and Efficient Use of Energy, Water and Natural Resources (SEWAN) conference, Tomsk, Russia, 14-16 November 2018.
9	**Fan YV,** Introduction and Application of P-graph Software in Municipal Solid Waste Management System, Invited speaker, School of Young Scientists “Methodology for the management of energy efficiency and resource saving” 13 November 2018, Tomsk, Russia
10	**Fan YV,** Klemeš JJ, Perry S, Lee CT, The Greenhouse Gas Emission of Different Waste Treatment Alternatives for Municipal Solid Waste, 13th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES2018), Palermo, Italy, 20 September - 4 October 2018.
11	**Fan YV,** Klemeš JJ, Walmsley TG, Lee CT, Perry S, Assessment of Waste Treatments for Municipal Solid Waste: P-graph. 2nd International Conference on Bioresources, Energy, Environment and Materials Technology, Seoul, Korea, 10-13 June 2018.
12	**Fan YV,** Klemeš, JJ, Chin HH, Extended Waste Management Pinch Analysis (E-WAMPA)

	Minimising Emission of Waste Management: EU 28, The 14th International Congress on Chemical and Process Engineering, **Bologna, Italy**, 26-19 May 2019.
13	**Fan YV,** Klemeš, JJ, GHG Emissions of Incineration and Anaerobic Digestion: Electircity Mix, 4th International Conference of Low Carbon Asia and Beyond (ICLCA 2018), **Johor Bahru, Malaysia,** 24-26 October 2018.
14	**Fan YV,** Klemeš JJ, Efficiency of pre-treatment for anaerobic digestion of lignocellulosic and municipal solid waste, XI International Conference on Computational, Heat, Mass and Momentum Transfer (ICCHMT 2018), **Krakow, Poland**, 21-24 May 2018. [Poster]
15	**Fan YV,** Klemeš JJ, Lee CT, Pre-and Post-Treatment Assessment for the Anaerobic Digestion of Lignocellulosic Waste: P-graph, 3rd International Conference of Low Carbon Asia and Beyond (ICLCA 2017), **Bangkok, Thailand**, 30-4 November 2017
16	**Fan YV,** Klemeš JJ, Lee CT, Challenges of Energy Efficiency Improvement for Anaerobic Digestion 20th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction (PRES'17), **Tianjin, China**, 21-24 August 2017;
17	**Fan YV,** Klemeš JJ, The Environmental Footprints and Available Handling for Cigarette Butts, 12th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES2017), **Dubrovnik, Croatia**, 4-9 October 2017;
18	**Fan YV,** Klemeš JJ, Lee CT, The update of anaerobic digestion and the environment impact assessment research, 13th International Conference on Chemical and Process Engineering, **Milano, Italy**, 28-31 May 2017;
Co-author of Plenary and Invited Lectures	
1	Klemeš JJ, **Fan YV,** Sustainability in a Multidisciplinary Scenario: Development of Circular Economy and Smart Cities, 8 December 2018, Plenary lecture, 4th ASIA International Conference, Langkawi, Malaysia.
2	Klemeš JJ, **Fan YV,** Environmental Footprints Assessment for Circular Economy and Smart Cities, 27 February 2019. Invited lecture, Fujian Normal University, Fuzhou, China
3	Klemeš JJ, **Fan YV.** The role of Energy Footprints to Reduce Emissions and Effluents and to support the Support Circular Economy. Plenary Lecture, Proceedings of the International Conference on Innovative Applied Energy – IAPE2019, Oxford, United Kingdom.
4	Klemeš, J.J., **Fan, Y.V.** Smart Cities Potential for Reducing the Environmental Footprints. Plenary Lecture, The First International Conference on Civil Engineering and Materials, National School of Applied Sciences Al Hoceima, Oujda, Morocco. 12 May 2017
5	Klemeš, J.J., **Fan, Y.V.,** Lee, C.T., Varbanov, P.S. Extending Process Integration to Sustainable Smart Cities. Plenary lecture, 3rd International Conference on Science, Engineering and the Social Sciences, Universiti Teknologi Malaysia, Johor Bahru, Malaysia, 17 May 2017
6	Klemeš, J.J., **Fan, Y.V.,** Environmental Footprint Reduction of Biowaste, Plenary lecture,Hong Kong Polytechnic University, Hong Kong – China, 27 May 2017

7	Klemeš, J.J., **Fan, Y.V.,** Lee C. T., Varbanov, P.S. Extending Process Integration to Sustainable Smart Cities, Invited lecture, Energy, Ecology and Environment (ICEEE2017), Stockholm, Sweden. 26 July 2017
8	Klemeš, J.J., Varbanov, P.S., **Fan, Y.V.** Sustainability and Complex Systems Thinking-Process Cities and Regions Integration. Plenary lecture, 3rd Cities Development and Ecological Management Conference & International Workshop on Urban Development and Ecological Management, Beijing Normal University, Beijing, China. 28 August 2017
9	Klemeš, J.J., **Fan, Y.V.,** Varbanov, P.S., Smart Cities Potential for Reducing the Environmental Footprint. Invited lecture, King Mongkut's University of Technologi Thonburi, Bangkok, Thailand. 31 October 2017
10	Klemeš, J.J., **Fan, Y.V.** New Views on De-carbonisation: Good and Bad Carbon. Plenary lecture, 3rd Int Conference of Low Carbon Asia and Beyond (ICLCA 2017), Bangkok, Thailand. 02 November 2017
11	Klemeš, J.J., **Fan, Y.V.,** Varbanov, P.S. Environmental Impact Assessment Quantification by Analysing the GHG and Smog/Haze Footprints, (CO2, CH4, NOx, SOx, VOC, PM), Indoor Air Quality and VOC Clean Technology WS. Invited lecture Hanyang University, Seoul, Republic of Korea. 21 November 2017
12	Klemeš, J.J., **Fan, Y.V.,** Varbanov, P.S. SPIL Research Targets: Integration of Processes and Environmental Objects – Management and Sustainable Society, Plenary lecture 3rd Asia International Conference, KLCC, Kuala Lumpur, Malaysia. Plenary Lecture. 09 December 2017
13	Klemeš, J.J., Varbanov, P.S., **Fan, Y.V.,** Energy and Water Footprints Reduction and Virtual Footprints Interactions., Invited lecture, University of Miskolc., Hungary. 13 March 2018
14	Klemeš, J.J., Varbanov, P.S., **Fan, Y.V.** Energy and Water Footprints Reduction and Virtual Footprints Interactions. Invited lecture, Faculty of Business Economics in Košice, Slovakia. 15 March 2018
15	Klemeš, J.J., **Fan, Y.V.,** Varbanov, P.S. Energy and Water Footprints as a Tool to reduce Emissions and Effluents to support Circular Economy. Plenary lecture, Taiwan 2018 International Symposium on the Circular Economy, Chemical Industry, and Tax policy, National Chengchi University, Taipei, Taiwan, Distinguished Keynote Speech. 02 April 2018
16	Klemeš, J.J., **Fan, Y.V.,** Varbanov, P.S., Process integration and energy saving, Plenary lecture, XI International Conference on Computational Heat, Mass and Momentum Transfer ICCHMT 2018 Conference, Cracow, Poland. 23 May 2018
17	Klemeš, J.J., **Fan, Y.V.,** Varbanov, P.S., Sustainability and Complex Systems Thinking to Deal with the Global Warming – Process Integration Extensions and Environmental Footprints Implementation, Plenary lecture, 7th Global Conference on Global Warming (GCGW-2018), Izmir, Turkey. 26 June 2018
18	Klemeš, J.J., **Fan, Y.V.,** Energy and Water Footprints to Support Circular Economy and Smart Cities. Plenary lecture, BWR 2018 Conference Plenary Lecture, Education University of Hong Kong, Hong Kong, China. 17 December 2018

19	Klemeš, J.J., **Fan, Y.V.** Internet of Things for Green Cities Transformation: Benefits and Challenges, Plenary lecture, 4th International Conference on Smart and Sustainable Technologies, Bol and Split, Croatia, 18 June 2019
20	Klemeš, J.J., **Fan, Y.V.,** Chin H.H., Circular Economy Sustainable Production Strategies for Chemical and Petrochemical Companies, Plenary lecture, 2019 Taiwan Chemical Industry Forum, International Convention Centre Taipei, Taiwan, ROC, 22 August 2019
21	Klemeš, J.J., Fan, Y.V Circular Economy, Energy Efficiency and Environmental Safety in Chemical Industry, Invited Keynote Lecture Section 4, XXI Mendellev Congress, Moscow, Russian Federation, 11 September 2019.