Essays on Sustainable Operations Management

by

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT
OF THE REQUIREMENTS FOR THE DEGREE OF

Doctor of Philosophy

in

THE FACULTY OF GRADUATE AND POSTDOCTORAL STUDIES
(Business Administration)

The University of British Columbia
(Vancouver)

July 2020

The following individuals certify that they have read, and recommend to the Faculty of Graduate and Postdoctoral Studies for acceptance, the thesis entitled:

Essays on Sustainable Operations Management

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Abstract

This dissertation comprises three independent essays on sustainable operations management.

In the first essay, we consider supply chains with joint production of carbon emissions, operating under either a carbon tax or an internal carbon pricing regime. Supply chain leaders, such as Walmart, are assumed to be environmentally motivated to induce their suppliers to abate their emissions. We derive a footprint-balanced scheme for reapportioning the total carbon emissions amongst the firms in the supply chain. This allocation scheme, which is the Shapley value of an associated cooperative game, is shown to be transparent and easy to compute. Further, when the abatement cost functions of the firms are private information, it incentivizes suppliers to exert pollution abatement efforts that minimize the maximum deviation from the socially optimal pollution level. Finally, it is the unique allocation mechanism satisfying certain contextually desirable properties.

The second essay analyzes a Canadian federal mandate to factor in upstream emissions during the environmental impact assessment of fossil fuel energy projects. We employ a cooperative game-theoretic model and propose the nucleolus mechanism to apportion upstream emission responsibilities. The nucleolus allocation avoids the distortionary effects of double counting and exhibits a certain contextually desirable consistency property. We develop a polynomial-time algorithm to compute the nucleolus and further provide an implementation framework in terms of two easily stated and verifiable policies. We also provide lower-bound guarantees on the welfare gains it delivers to firms and on the incentives it offers them to adopt emission abatement technologies.

In the third essay, we consider the operations of bike-sharing systems. Despite their growing popularity as a sustainable urban transport option, bike-share programs in several cities such as Seattle and Montreal have run into financial difficulties due to low ridership and high operational costs. Further, their environmental benefits are ambiguous since a majority of users are observed to substitute from public transport or walking. We develop a consumer transport mode choice model to analyze the economic and environmental implications of three key operational levers: the pricing structure, station coverage and density, and frequency of rebalancing operations.

Lay Summary

In response to the increasing threat of global climate change, governments in several regions have begun to institute new environmental regulations, such as carbon taxes, upon businesses. In parallel, green business models have also emerged that attempt to align profit motives with environmental objectives. This dissertation is comprised of three essays: in the first two, we examine environmental regulations placed on supply chain emissions, and in the third essay, we examine a novel green business model of bike-sharing. Employing game-theoretic methods and case studies, we analyze these regulations and the bike-sharing business model along economic and environmental dimensions. The primary objective of this dissertation is to develop and apply analytical tools to aid in the design of better regulations and business models that can achieve the desired environmental objectives while minimizing and distributing the economic burden fairly.

Preface

Versions of Chapters 2 and 3 have been submitted for publication. Chapter 4 will be reformatted and submitted for publication.

Chapter 2 is co-authored with Professors Daniel Granot, Frieda Granot, Greys Sošić, and Hailong Cui. Chapters 3 and 4 are co-authored with Professors Daniel Granot and Frieda Granot. In all chapters, I was a primary contributor and I was involved in developing the models, carrying out the analysis, and reporting the results, as presented in this dissertation. Therefore, I also assume full responsibility for editorial and technical mistakes, if any are found. However, at the same time, all my co-authors have provided invaluable intellectual guidance and devoted tremendous time and effort on these projects.

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Acknowledgments

I am deeply grateful to my advisors, Professor Daniel Granot and Professor Frieda Granot, for their constant support, patience, and encouragement. Their expertise, attention to detail, and the academic freedom they provided made my PhD an enriching intellectual experience. I have benefited immensely from their wise mentorship, the lessons of which extend across all spheres of academic life.

I want to thank Professor Mahesh Nagarajan for his guidance, and the time and effort he expended towards making me a better researcher. His support has played a huge role in my academic development and for this, I am immensely grateful to him.

I also thank my committee member, Professor Werner Antweiler, for his useful feedback on my projects. His course on environmental management shaped the direction of this thesis. I am grateful to Professor Dale Griffin for his contributions to my academic training. I would also like to thank Professor Tim Huh, Professor Harish Krishnan, and Professor Hasan Cavusoglu. The perspectives I gained from them on research and teaching were truly valuable. Thanks are also due to Elaine Cho and Rita Quill for enabling a conducive academic environment.

I must thank several of my fellow graduate students at the Sauder School of Business for their friendship and the many wonderful conversations which made my time at UBC that much more enjoyable.

Finally, and most importantly, my deepest gratitude is towards my parents, my brother, and Lavisha. This journey would not have been possible without their unconditional love over the years.

Chapter 1

Introduction

A global consensus has evolved gradually around the need to balance economic growth with environmental sustainability. Recently, in response to the impending risks due to climate change, the 2015 Paris Climate Agreement sets out an objective to pursue efforts to limit the temperature increase to 1.5°C above pre-industrial levels (Paris Agreement 2015). To achieve this objective, the United Nations Environment Programme (UNEP 2019) finds that a 7.6% year-over-year reduction in global annual emissions is necessary. This changing landscape has required existing businesses to move beyond solely focusing on economic profitability and to also consider the environmental aspects of their operations. It has also, in some cases, facilitated the growth of entirely new sustainable business models such as the sharing economy.

The field of sustainable operations management similarly integrates considerations of environmental sustainability within traditional lines of enquiry, as well as, explores new avenues of research. It thereby plays a critical role in identifying business and policy solutions for environmental challenges. As identified by Atasu et al. (2020), two major themes of research within sustainable operations management have been: (i.) operations management for a low-carbon economy, and (ii.) sustainable business model innovation. The former stream studies the optimal design of regulations such as carbon accounting, carbon taxes, cap-and-trade etc. and their impacts on firms operational decisions and adoption of cleaner technologies (see, for example, Caro et al. 2013, Jira and Toffel 2013, Plambeck and Taylor 2013, Sunar and Plambeck 2016, Drake 2018). The latter stream considers the operational design and environmental outcomes of novel business models such as, for example, online grocery (Belavina et al. 2016), and sharing economy models (Bellos et al. 2017, Agrawal et al. 2019, Orsdemir et al. 2019).

This thesis comprises of three independent essays. The first two essays broadly fall under the first theme of designing better policies or regulations that suitably incentivize firms to achieve desired environmental objectives. The third essay on bike-sharing business models follows the second theme.

Greenhouse gas emissions from the supply chains of just the 2,500 largest global corporations account for more than 20% of global emissions. Further, the direct emissions of firms account for only about 14% of their total emissions with the rest of it coming from their supply chains (Matthews et al. 2008). Therefore, rationalizing emissions in supply chains could make an important contribution towards meeting the global CO_2 emission reduction targets tied to the 2015 Paris Climate Agreement. This motivates our first essay where we consider supply chains with joint production of GHG emissions. That is, supply chains wherein the actions of an individual firm influences not only its own direct emissions but also influences emissions at other stages in the supply chain. This is often the case in practice. We suppose that the leader of such a supply chain (for example, Walmart) is environmentally motivated and strives to reduce supply chain emissions. The supply chain leader identifies joint responsibilities, in view of the ability of firms to directly or indirectly influence the emissions of various processes in the supply chain, and apportions the net supply chain emissions amongst the constituent firms by leveraging its knowledge. The supply chain leader's objective is to incentivize firms to exert suitable actions that reduce the overall supply chain emissions. The supply chain leader, in our model, aims to do so by redistributing the total carbon tax burden on the supply chain, in view of the joint responsibilities for emissions. We adopt a cooperative game theory methodology to derive a fair and transparent scheme for apportioning the total carbon emissions in the supply chain, which is shown to incentivize firms to exert, in some sense, optimal abatement efforts to reduce their pollution. Via a case study based on the Walmart-Nautica jeans' supply chain, we illustrate how our proposed emission re-apportionment mechanism could be implemented by supply chain leaders to achieve supply chain emission reductions.

In the second essay, we focus on a recent Canadian environmental regulation directed at proposed energy projects. Faced with increasing stakeholder pressure from environmental thinktanks and NGOs, the Canadian federal government announced on January 27, 2016 that the energy regulator, National Energy Board, later superseded by the Impact Assessment Agency of Canada, would factor in upstream emissions during the environmental impact assessment stage for proposed energy projects (Canada 2016). This has significant implications for several pipeline projects across Canada (such as the Trans Mountain pipeline expansion) that transport crude oil or refined products to refineries and shipping terminals, and other energy projects. The upstream emissions attributable to a proposed project could be compared against a rejection threshold level of emissions whereby the regulator sets a predetermined level of upstream emissions beyond which the project will be rejected (Schaufele 2016), or as in the case of the approval granted to the Trans Mountain pipeline project, the regulator could also require the firm to offset some or all of the associated upstream emissions.

However, a rejection threshold policy or offset requirements that take into account all upstream emissions of an energy project would have to be calibrated, depending on the stage of the supply chain the project is situated at, or otherwise it risks inducing distortionary effects by favouring upstream energy projects over more downstream ones. This is primarily a consequence of double counting by attributing to each entity in the supply chain all associated upstream emissions. We address these concerns and develop an emission responsibility accounting mechanism for energy supply chains that avoids the distortionary economic effects of double counting while embodying the principle of upstream emission responsibility mandated by the Canadian federal government. Furthermore, the mechanism we propose exhibits a consistency property that is especially important in a regulatory context wherein energy supply chains span multiple legal jurisdictions. We also provide a simple implementation framework for our proposed mechanism in terms of two easily stated and compliance-verifiable policies. Our results could be of interest to energy regulators and energy companies aiming to strike a balance between energy and economic needs and environmental concerns. They imply that a mandated, centrally determined and binding emission responsibility allocation scheme can be replaced, in some sense, by a decentralized scheme that provides a degree of freedom to entities in energy supply chains to collectively arrive at an apportionment of pollution responsibilities that is beneficial from the entire supply chain's perspective. Such a decentralized policy framework, that calls upon supply chain entities to collaborate with their partners, may also catalyze ancillary environmental benefits. Importantly, we contextualize our discussion with a case study on the proposed expansion of the Trans Mountain pipeline in Western Canada.

In the third essay, we focus on the operations of bike-sharing systems. Bike sharing programs have rapidly gained in popularity and a key reason being that they present a sustainable and green urban transport option complementing the existing modes of transport. Despite the growing popularity of bike sharing, systems in several major cities, such as Seattle's Pronto and Bixi in Montreal, have run into financial difficulties. High operational costs arising from system rebalancing, theft and vandalism, coupled with lower than projected levels of ridership are commonly identified as the major contributing factors.

On the other hand, the environmental benefits of a bike-sharing program, as a consequence of reduced vehicular emissions from individuals substituting away from personal automobiles, might be less substantial than presumed. For example, the 2014 survey report of the Capital Bike Share Program in Washington D.C. notes that - "40% percent of respondents would have ridden a bus or train if Capital Bikeshare had not been available for the most recent trip, another 37% would have walked to their destination, only 12% of respondents would have driven or ridden in a car." Another survey of bike-share users in Portland estimated that only up to a quarter of the users had substituted away from cars. Further, typically the rebalancing operations are carried out with trucks which results in significant carbon emissions. Both these factors suggest that in certain cases, the environmental benefits of bike-sharing programs might be overstated. Lending further evidence, Fishman et al. (2014), using surveys and bike trip data, study the environmental impact of bike share programs across four cities world-wide, and find that the London bike-share system had a net negative environmental impact.

This motivates our third essay where we consider three key strategic and operational decisions faced by bike share operators - the coverage and density of the system, the pricing model and the frequency of rebalancing. Our objective is to provide insights to planners to design bike-sharing systems that are financially viable with high ridership and low operational costs, which maximize environmental benefits.

Chapter 2

Incentives and Emission Responsibility Allocation in Supply Chains

2.1. Introduction

In view of the urgency and challenges of mitigating climate change, it should be noted that greenhouse gas (GHG) emissions from the supply chains of the 2,500 largest global corporations accounts for more than 20% of global GHG emissions (van Hoek et al. 2019). Further, typically, the emissions associated with the direct operations of a company are far exceeded by the indirect emissions associated with its supply chain. Indeed, the average ratio of supply chain to direct carbon emissions is 5.5, and for the retail sector, this ratio is much higher at 10.9 (Carbon Disclosure Project (CDP) 2019[1]). Therefore, accounting and rationalizing emission responsibility in supply chains could make an important contribution to achieving the desired global CO_2 emission reduction targets (Paris Agreement 2015[2]).

Increased attention, visibility, and stakeholder pressures, have motivated several organizations to integrate environmental concerns in the formal and informal governance of their supply chains (Huang et al. 2019). Walmart is one of the companies that has embraced its responsibility to protect the environment and reduce emissions in its vast supply chain. To act upon its environmental goals, Walmart, since 2007, has started to collect data to assess GHG emissions of its supply chain. To facilitate the rationalization of its supply chain, Walmart is collaborating with academics and environmental third-party groups to identify processes in its supply chain that generate significant carbon emissions (Oshita 2011, Plambeck 2012). The United States federal government followed suit in 2009, when a new Presidential Executive Order required federal agencies to set reduction targets and track the reduction of

[1] https://www.cdp.net/

[2] https://treaties.un.org/pages/ViewDetails.aspx?src=TREATY&mtdsg_no=XXVII-7-d&chapter=27&lang=en

GHG emissions, including those associated with their supply chains[3], and many corporations have similarly joined the efforts to collect information about their GHG emissions. The CDP Supply Chain Program is a collaboration of multinational corporations that have requested information about their key suppliers' GHG emissions as well as their vulnerabilities and opportunities associated with climate change.

It is well recognized that the actions of an individual firm in a supply chain, aside from being responsible for its own direct emissions, can often influence emissions at other stages in the supply chain. As an example, the packaging design choice by a manufacturer is likely to impact the distributor's transport emissions. Similarly, in the oil industry, the choice of crude oil blends and diluents added at the extraction stage affects emissions associated with shipping and transportation across oil pipelines, as well as emissions during the refining stage (ICCT 2014). Therefore, to improve environmental performance, motivated supply chain leaders need to understand the interrelated sources of emissions in their supply chains. In particular, to incentivize firms to reduce overall supply chain emissions, suppliers should be held responsible both for their own direct emissions, as well as for emissions by other firms, which they can jointly reduce. That is, aside from direct emission responsibility, supply chain leaders should attribute indirect emission responsibilities to firms which can lower emissions at other stages in the supply chain by, e.g., expertise and innovation sharing, or by modifying their operational decisions, product design, material selection, or packaging design (see, e.g., Benjaafar et al. 2013, Gallego and Lenzen 2005, LS & Co. 2017, HP Living Progress Report 2014[4], and Herman Miller 2016[5]).

Recognizing the urgency of mitigating climate change, more than 60 regional and national governments have implemented policies that price carbon emissions[6]. In that respect, our essay can be viewed as modeling the challenges and opportunities facing supply chain leaders operating under a carbon tax regime, wherein a regulator levies a penalty on the emissions generated by the firms in the supply chain. The supply chain leaders, such as Walmart, are assumed to be environmentally motivated whose objective is to incentivize constituent firms to reduce the overall supply chain emissions. In the presence of a carbon tax regime, they aim to achieve this objective by leveraging their knowledge on the sources of pollution, and redistributing the total carbon tax burden among the firms in the supply chain.

We note, however, that it has been suggested, e.g., by Aldy and Gianfrate (2019), that even companies operating in areas without carbon tax legislation must prepare for potential increases in their operating costs due to carbon prices. Companies in such settings can benefit

[3]https://www.whitehouse.gov/the-press-office/president-obama-signs-executive-order-focused-federal-leadership-environmental-ener.

[4]http://www8.hp.com/h20195/v2/GetDocument.aspx?docname=c04152740

[5]http://www.smartfurniture.com/hermanmiller/environmental.html

[6]https://carbonpricingdashboard.worldbank.org/map_data

by using internal carbon pricing as it helps them to measure and manage risks associated with existing pricing regimes and to identify risks and opportunities and use them to adjust their strategies. For example, in 2012, Microsoft implemented an internal carbon-pricing system that assigned responsibilities to each unit for their direct and indirect carbon emissions. In 2020, Microsoft is doubling up on their efforts to mitigate emissions[7], and aim, for example, to cut their carbon emissions, direct and the entire supply chain's, by more than half by 2030. In July 2020, Microsoft will start phasing in their current internal carbon tax of \$15/metric ton, to cover all Scope 1 (direct and on-site), 2 (indirect from energy usage) and 3 (other indirect) emissions. Moreover, as clarified by Microsoft, "Unlike some other companies, our internal carbon tax isn't a 'shadow fee' that is calculated but not charged. Our fee is paid by each division in our business based on its carbon emissions, and the funds are used to pay for sustainability improvements". Thus, our essay can also be viewed as modelling the challenges and opportunities facing firms such as Microsoft, that aim to implement effective internal carbon pricing in their supply chains to achieve sustainability objectives and to generate funds for sustainability projects.

We adopt a cooperative game theory methodology to derive a fair and transparent scheme for apportioning the total GHG emissions in the supply chain, which is shown to incentivize firms to exert, in some sense, optimal abatement efforts to reduce their pollution. Indeed, we examine the problem of apportioning emission responsibility in supply chains from three different and complementary perspectives. Firstly, we consider the application of cooperative game theory methodology to our setting, and in particular, the Shapley value, a commonly used allocation method. We then proceed to justify its suitability as an allocation mechanism in our context. In particular, we show that it belongs to the core of an associated cooperative game and, additionally, it is easy to compute (Theorem 2.1). As such, it overcomes the main drawback of the Shapley value for general cooperative games, stemming from its computational intractability in many cases. Secondly, we consider the incentives for emission abatement point of view, bearing in mind that Caro et al. (2013) showed that footprint-balanced allocation rules, i.e. rules that allocate precisely the entire pollution among the supply chain members, in general, cannot achieve first-best emission reduction efforts. Following their line of enquiry, we consider situations when footprint balance might be a natural requirement and are able to show that when the pollution abatement cost functions of the firms are private information, as is typically the case, the Shapley value incentivizes suppliers to exert pollution abatement efforts that, among all footprint-balanced allocation schemes, minimize the maximum deviation from the socially optimal pollution level (Theorem 2.4). Thirdly, we consider some potentially desirable properties that a pollution responsibility allocation mechanism should satisfy and discuss their implications on supply chain welfare

[7] https://blogs.microsoft.com/blog/2020/01/16/microsoft-will-be-carbon-negative-by-2030/

and implementation. We then demonstrate that the Shapley value is the unique allocation mechanism satisfying these properties (Theorem 2.6).

Finally, in this essay, we assume that the GHG emissions from all processes in the supply chain are known. We acknowledge, though, that there are numerous difficulties involved in calculating GHG emissions from all supply chain members. Nevertheless, consistent attempts are being made by firms to measure GHG emissions in their supply chains. Indeed, it is generally suggested that firms should follow the Corporate Accounting and Reporting Standard by the GHG Protocol[8], which clarifies the accounting methodology, and also provides examples of multiple firms, such as the Ford Motor Company, that have successfully implemented their emissions accounting procedures. It should be further noted in that regard that it was already reported several years ago (CDP 2011), that 75 multinational companies, such as Walmart, Dell, Amazon, Ford and Vivendi, have inquired with nearly 8,000 of their suppliers about their carbon emissions[9]. We also note that, for instance, Apple provides environmental reports for their products[10] which detail GHG emissions from different stages in a product's lifecycle, Timberland provides "green index" for their products,[11] which details GHG emissions, chemicals used, and resource consumption, and the Innovation Center for U.S. Dairy provides emissions for fluid milk and other dairy products. Good illustrative examples of calculating the carbon footprint at different parts in the supply chain are provided, for example, by the New Belgium Brewing Company for a 6-pack of their Fat Tire Amber Ale[12] and by Levi's and their 501 jeans[13].

The plan of the essay is as follows. In §2.2, we provide a brief literature review. In §2.3, we present our two-stage model and adopt a cooperative game-theoretic approach for the second-stage supply chain emission responsibility apportionment, to be referred to as the GREEN game. In §2.4, we consider the emission abatement incentives offered to the firms in the first-stage, in a setting wherein the abatement costs are private information to the firms, and reveal the ability of the Shapley allocation to incentivize suppliers to exert, in some sense, optimal abatement efforts. In §2.5, we present some additional contextual desirable properties satisfied by the Shapley allocation, which are then used to develop two characterizations for the Shapley mechanism to allocate emission responsibilities in supply chains. We perform a case study in §2.6 on the Walmart-Nautica jeans supply chain to contextualize our results. Finally, some concluding remarks are provided in §2.7. All proofs are presented in Appendix A.

[8] https://ghgprotocol.org/corporate-standard

[9] http://www.prnewswire.com/news-releases/companies-blind-to-climate-risks-in-half-their-supply-chains-finds-largest-global-study-300209209.html

[10] http://www.apple.com/environment/reports/

[11] http://greenindex.timberland.com

[12] http://www.newbelgium.com/Files/the-carbon-footprint-of-fat-tire-amber-ale-2008-public-dist-rfs.pdf

[13] http://levistrauss.com/wp-content/uploads/2015/03/Full-LCA-Results-Deck-FINAL.pdf

2.2. Literature Review

Our work is broadly related to two streams of literature. Firstly, there is a growing area of study concerning sustainable supply chain management, and in particular, supply chain emission accounting and apportioning of shared emissions. Gallego and Lenzen (2005) are primarily concerned with allocations of GHG emission responsibilities which are footprint balanced. Their non-game-theoretic model has some features in common with our modelling framework. Specifically, somewhat similar to us, they suggest that GHG emission responsibilities should be shared among all supply chain members who have directly or indirectly created these emissions, and it can be shown that their allocations belong to the core of our GREEN game. Plambeck (2012) elaborates on some of the challenges facing firms that try to reduce their GHG emissions through operations and supply chain management, Sunar and Plambeck (2013) investigate three allocation methods of carbon emissions among co-products, Benjaafar et al. (2013) study the potential synergies and emission reductions from cooperation in a supply chain (see also Chen et al. 2019) and Corbett and DeCroix (2001), and Corbett et al. (2005) study shared-savings contracts in supply chains and their environmental impact.

Caro et al. (2013) study a similar process-based model of joint production of GHG emissions in a supply chain wherein the total emissions can be decomposed into processes, and each process possibly influenced by a number of firms, and focus on the incentives induced by emission allocation mechanisms. Their modelling framework for identifying joint responsibility is identical to ours and from an emission abatement incentives perspective, our approach to induce optimal abating efforts by firms in a supply chain can be viewed as complementary to that of Caro et al. (2013). Specifically, when a central planner allocates emissions to individual firms in the supply chain and imposes a cost on them proportional to the emissions allocated, they find that even if the carbon tax is the true social cost of carbon, emissions need to be over-allocated to induce optimal effort levels. However, as noted by the authors, while double counting may be feasible to implement in vertically integrated firms, "regulators and supply chains are unlikely to implement incentive mechanisms based on extensive double counting". In fact, to avoid double counting, the GHG Protocol advises that "companies should take care to identify and exclude from reporting any Scope 2 or Scope 3 emissions that are also reported as Scope 1 emissions by other facilities, business units, or companies included in the emissions inventory consolidation."

We therefore address the complementary question and investigate the impact on emission abating efforts of allocation rules which, by contrast, are restricted to be footprint-balanced. Specifically, we show that when firms' abating cost functions are private information, then, restricted to footprint-balanced linear allocation rules, the Shapley value allocation induces abating efforts which minimize the maximum deviation from the socially optimal pollution level (Theorem 2.4).

Secondly, we also contribute to the literature on cooperative game theory and its applications in operations management. Cooperative game theory finds applications in several allocation problems in supply chains (see Nagarajan and Sošić 2008, for a review). In particular, the Shapley value has been applied as a profit or cost-sharing mechanism in transhipment (e.g., Granot and Sošić 2003, and Sošić 2006), inventory pooling (Kemahlioğlu-Ziya and Bartholdi 2011) and information sharing in supply chains (Leng and Parlar 2009).

Our work is also related to a branch of the game-theoretic literature concerned with cost allocation problems on graphs. Indeed, our GREEN game model can be shown to be a generalization of the tree game model (Megiddo 1978), which in turn is an extension of the airport game, e.g., Littlechild and Owen (1973), wherein airport landing fees have to be allocated among airlines using a common runway. The class of highway games (e.g., Çifçi et al. 2010), wherein players are responsible for the cost associated with an arbitrary but contiguous set of arcs in a weakly acyclic graph, can also be viewed as a generalization of airport games.

Finally, we note that our work is also related to the extensive literature on carbon border adjustments in environmental economics (Eyland and Zaccour 2014, Larch and Wanner 2017, Böhringer et al. 2015, Kortum and Weisbach 2017). The practical administrative issues pertaining to carbon border adjustments addressed in this stream of literature such as the (i) difficulties associated with estimating the embodied emissions in supply chain trade, (ii) the cost of obtaining this information from suppliers, and (iii) the possibility of supplier misrepresentation, also concern our work.

2.3. The GREEN Game Model

We consider a supply chain consisting of several firms, such as suppliers, manufacturers and assemblers, who are cooperating in the joint production of a final product or products. We model joint production in the supply chain as in Caro et al. (2013) and Battaglini (2006). We denote the set of firms in the supply chain by $N = \{1, \ldots, n\}$, and $M = \{1, \ldots, m\}$ is the set of distinct processes in the supply chain. Let $f = [f_1, \ldots, f_m]$ denote the total supply chain carbon footprint vector consisting of the emissions associated with all processes in the supply chain. The carbon emission, f_j, at each process j can be jointly influenced by the actions undertaken by some subset of firms $N^j \subseteq N$. For example, the emissions at the transportation stage in a supply chain will be directly influenced by the operational decisions made by the distributor, but could also be lowered by an assembler, who is packaging the products more efficiently. We consider a firm i to be directly or indirectly responsible for the pollution at a process j if its actions could influence the emissions, f_j. Following Caro et al.

(2013), we therefore represent the responsibilities of the firms for the pollution of the various processes in the supply chain by a $(0,1)$-matrix, $\mathbf{B} = (b_{i,j})$, for $i \in N$ and $j \in M$, where $b_{i,j} = 1$ for $i \in N$ and $j \in M$, if and only if $i \in N^j$.

We suppose that the supply chain is operating under a carbon tax regime wherein a regulator levies a carbon penalty denoted by $p^S > 0$ per ton of carbon emissions in the supply chain. Further, we assume that the supply chain leader, such as Walmart, is motivated to reduce emissions in their supply chains. The supply chain leader strives to do so by leveraging its knowledge reflected by the matrix $\mathbf{B}$, about the joint responsibilities for pollution in the supply chain. The supply chain leader aims to identify a pollution allocation rule to apportion the total emissions, $\sum\limits_{j \in M} f_j$, of the supply chain, in a manner which leverages its insight about joint pollution responsibilities, so as to incentivize firms to take suitable actions to reduce the total supply chain emissions. Formally, a pollution allocation rule ϕ is defined on the set of firms N, set of processes M, and the responsibility matrix B. Then, the allocation rule ϕ is a function $\phi(\mathbf{B}, f)$ which allocates to each firm, i, its total pollution responsibility, $\phi_i = \phi_i(\mathbf{B}, f)$, such that $\sum\limits_{i=1}^{n} \phi_i = \sum\limits_{j=1}^{m} f_j$.

The supply chain leader in Caro et al. (2013) is also assumed to be motivated by environmental concerns. However, in their model, the supply chain leader voluntarily decides to offset the supply chain emissions and then can, via payments, incentivize supply chain partners to reduce their emissions. In contrast, in our model, the role of the supply chain leader is more limited. Its objective continues to be achieving lower supply chain emissions. However, it aims to do so by leveraging its knowledge about the joint production of pollution, while redistributing the total carbon tax burden on the supply chain.

Our model can be interpreted as a two-stage model with the following sequence of decisions in each stage:

Stage 1: Each firm i in the supply chain exerts efforts towards reducing emissions, f_j, of those processes j that it can influence, i.e., $i \in N^j$.

Stage 2: The net supply chain emissions, $\sum\limits_{j \in M} f_j$, are allocated amongst the supply chain firms according to the predetermined allocation mechanism, $\{\phi_i\}_{i \in N}$, such that $\sum\limits_{i \in N} \phi_i = \sum\limits_{j \in M} f_j$. Then, from each firm i, the corresponding carbon penalty, $p^S \phi_i$, is collected.

The allocation mechanism adopted in the second-stage will naturally affect the incentives offered to firms to exert efforts to abate emissions in the first stage. In the remainder of this section, we therefore, address the problem of allocating emissions to firms in the supply chain. To that end, we employ cooperative game theory methodology to formally consider the allocation of the total supply chain emissions, $\sum\limits_{j \in M} f_j$, among the constituent firms.

2.3.1 Cooperative Game Definitions and Model

To present our game-theoretic formulation, we first introduce some definitions and notation. A *(cost) cooperative game* in a characteristic function form is the pair (N, c), where N is the set of players and c is the characteristic function such that for each $S \subseteq N$, $c(S)$ is the cost that can be attributed to S. The *core*, $\mathcal{C}((N, c))$, of a game (N, c) is one of the most fundamental solution concepts. It consists of all vectors $x = (x_1, x_2, \ldots, x_n)$ which allocate the total cost, $c(N)$, among all players in N such that no subset of players, S, is allocated more than the cost, $c(S)$. Formally, $\mathcal{C}((N, c)) = \{x \in \mathbb{R}^n : x(S) \leq c(S), \forall S \subset N, x(N) = c(N)\}$, where $x(S) = \sum_{j \in S} x_j$. The core of a game could be empty, and if non-empty, it usually does not consist of a unique allocation vector. The characteristic function of a game (N, c) is said to be *concave* if $c(S \cup \{i\}) - c(S) \leq c(Q \cup \{i\}) - c(Q)$ for all $i \notin S$ and $Q \subseteq S \subseteq N$. The game (N, c) is said to be *monotone* if for all $Q \subseteq S \subseteq N, c(Q) \leq c(S)$, and is said to be *concave* if its characteristic function, c, is concave. The core of a monotone game, if not empty, consists only of non-negative allocation vectors and the core of a concave game is non-empty (Shapley 1971).

We now specialize the above development to our particular context of apportioning emissions in a supply chain. The set of players, N, consists of all members of the supply chain, "costs" are replaced with "emissions", and for a set of firms S, let $b_{S,j} = 1$ if at least one firm in S is responsible for the pollution of process j, i.e., if $b_{i,j} = 1$ for some $i \in S$, and 0 otherwise. Then, the total pollution, $c_G(i)$, that can be attributed, perhaps not exclusively, as the responsibility of player i is given by,

$$c_G(i) = \sum_{j \in M} f_j b_{i,j}. \tag{2.1}$$

Similarly, the total pollution, $c_G(S)$, that can be attributed to a subset of firms, S, perhaps not exclusively, is given by,

$$c_G(S) = \sum_{j \in M} f_j b_{S,j}. \tag{2.2}$$

Then, the total pollution that has to be allocated to all firms in the supply chain is given by $c_G(N)$. We refer to the pair, (N, c_G), as the GHG Responsibility - Emissions and Environment (GREEN) game associated with the supply chain, where N is the set of players (i.e., firms), and the characteristic function[14] $c_G(S)$ is as defined above for all subsets S of

[14] Note that in GREEN games, as well as, e.g., airport games, highway games or related games such as those induced by joint cleaning a polluted river, $c(S)$ does not represent the "cost" that S would incur if it severed its cooperation with the rest of the players and acted alone, since the option of acting alone is not possible in these situations. That is, e.g., the option of constructing a different runway or highway serving only S is not feasible. In these situations, $c(S)$ was chosen in the literature to represent, e.g., either the cost that S would incur if it acted alone, or the cost it would have incurred *had* it been able to act alone, or some agreed upon

N.

Example 2.1. *To clarify the above discussion, consider $N = \{1, 2, 3\}$ to be the set of firms in a three-player supply chain, $M = \{m_1, m_2, m_3\}$ to denote the set of processes, and $f = [f_1, f_2, f_3]$ corresponds to the supply chain carbon footprint vector over the processes. Suppose that while firms 2 and 3 are individually responsible for pollution at processes m_2 and m_3, respectively, all three firms can jointly influence the emissions of process m_1. Therefore, the responsibility matrix is given by, $\mathbf{B} = (b_{i,j})$, where, $b_{1,1} = b_{2,1} = b_{3,1} = 1$, $b_{2,2} = b_{3,3} = 1$, while the rest of the entries in $\mathbf{B}$ are all 0. Denote the GREEN game by (N, c_G). Then, $c_G(\{1\}) = f_1$, $c_G(\{2\}) = c_G(\{1,2\}) = f_1 + f_2$, $c_G(\{3\}) = c_G(\{1,3\}) = f_1 + f_3$, $c_G(\{1,2,3\}) = c_G(\{2,3\}) = f_1 + f_2 + f_3$.*

Proposition 2.1. *The GREEN game (N, c_G) is concave.*

Proposition 2.1 implies that the core of (N, c_G) is non-empty. Further, it also implies that a commonly employed solution concept for general cooperative games, the Shapley value (Shapley 1953), belongs to the core.

2.3.2 The Shapley Allocation

The Shapley value (Shapley 1953), $\Phi(c)$, of a cooperative game, (N, c), is the unique allocation which satisfies the following axioms:

1. *Symmetry:* If players i and j are such that for each coalition S not containing i and j, $c(S \cup \{i\}) - c(S) = c(S \cup \{j\}) - c(S)$, then $\Phi_i(c) = \Phi_j(c)$.
2. *Null Player:* If i is a null player, i.e., $c(S \cup \{i\}) = c(S)$ for all $S \subset N$, then $\Phi_i(c) = 0$.
3. *Efficiency:* $\Sigma_N \Phi_i(c) = c(N)$.
4. *Additivity:* $\Phi(c^1 + c^2) = \Phi(c^1) + \Phi(c^2)$ for any pair of cooperative games (N, c^1) and (N, c^2).

It was shown by Shapley (1953) that $(\Phi_i(c))$, given by (2.3) below, is the unique allocation rule which satisfies the above four axioms.

$$\Phi_i(c) = \sum_{\{S : i \in S\}} \frac{(|S| - 1)!(n - |S|)!}{n!} \left(c(S) - c(S \setminus \{i\})\right). \tag{2.3}$$

upper bound for the cost that S should incur. In GREEN games, the value of $c(S)$ is induced by desirable regulations that view firms responsible for the pollution they create either directly or indirectly, which, in some sense, is an upper bound for the responsibility that should be attributed to S.

Note that the Shapley allocation provides a direct link between players' marginal contributions and their corresponding allocations. Young (1985) has provided an alternative axiomatization of the Shapley value wherein the additivity axiom is replaced with a compelling monotonicity axiom. In general, the Shapley value is perceived as a fair and "justifiable" allocation method, and it is not surprising that it was extensively considered as an allocation method in a variety of settings, including, in the airport game previously mentioned, for generating airport landing fees (Littlechild and Owen 1973).

We now provide a characterization of the Shapley value for GREEN games. We recall that for each process, $j, j \in M$, N^j denotes the set of firms that can affect the emissions of process j, i.e., $i \in N^j$ if and only if $b_{i,j} = 1$.

Theorem 2.1. *The allocation according to which the pollution, f_j, of each process j is allocated equally among all firms in N^j is the Shapley value of (N, c_G).*

Remark 2.1. *As noted previously, we assume that the emissions from all processes in the supply chain are measurable, and our primary focus is on the "second stage" problem of constructing a fair allocation mechanism which accounts for direct and indirect pollution responsibilities. However, we observe that Theorem 1 implies that the Shapley allocation is decomposable on the set of processes in the supply chain. This implies therefore that the lack of accurate information about emissions associated with certain processes in the supply chain shall not hinder the application of the Shapley allocation to the rest of the processes.*

By Theorem 2.1, the Shapley value of GREEN games is easy to compute and has a natural fairness property. Indeed, it can be viewed as a "common-sense" allocation mechanism that holds each firm equally responsible for the emissions of each process for which it is directly or indirectly responsible. Since, the abatement efforts exerted by the firms during the first-stage are typically non-verifiable and non-contractible, the Shapley allocation is only a function of the emissions themselves and not of the abatement efforts.

In the next section, we investigate the first-stage abatement decisions induced by the adoption of the Shapley allocation in the second stage to apportion supply chain emissions. Specifically, we demonstrate that the "common-sense" solution motivates, in some sense, optimal abating efforts by firms to reduce pollution. It is interesting to note that these results only depend on the expression of the Shapley allocation, as given by Theorem 2.1, and are independent of the GREEN game formulation, which yielded this allocation.

2.4. Footprint Balance and Emission Abatement Incentives

The choice of allocation mechanism employed in the second stage of our model will clearly influence the emission reduction efforts exerted by the firms in the first stage. As elaborated previously, in the second stage, we implicitly restrict our attention to allocation mechanisms that are footprint-balanced. Caro et al. (2013) demonstrate that footprint balanced allocation rules, in general, cannot achieve first-best emission reduction efforts. However, in certain situations footprint balancedness is an intrinsic constraint while designing a pollution allocation mechanism. Accordingly, we investigate in this section the first-stage pollution abatement incentives that can be generated by footprint balanced emission responsibility allocations. Specifically, in Theorem 2.4 we prove that, under some assumptions on the abatement cost functions, the Shapley allocation rule induces suppliers to employ abating efforts that minimize the maximum deviation from the socially optimal pollution level.

As will be clarified subsequently, one approach to prove Theorem 2.4, which we present in Appendix A, involves the application of the implicit function theorem. We note, however, that such an approach imposes some technical assumptions that could be difficult to verify, and which restrict the generality of the results derived. Therefore, we also present an alternate approach to prove Theorem 2.4, involving fewer technical assumptions, by following, and to some extent, extending the monotone comparative statics methods of Topkis (1978, 1998), and Milgrom and Roberts (1990). Our extension is of independent interest with potential applications in equilibrium analyses of other game theoretic models of supply chains.

In the next subsection we develop the monotone comparative statics results which will be subsequently used to prove Theorem 2.4.

2.4.1 Generalized Comparative Statics

In the following discussion, we closely follow the notation and definitions of Topkis (1998) and Jensen (2018). Consider an objective function $u(x,t)$, where $t \in T$ is a vector of parameters, $x \in X \subseteq \mathbb{R}$ is a single-dimensional decision variable, X is convex, and T is a convex subset of a real vector space. Let $G(t)$ denote the set of maximizers for the following optimization problem, and assume that all maxima are interior points in X,

$$G(t) = \arg\max_{x \in X} u(x,t). \tag{2.4}$$

A real-valued function $f(x)$ with $x \in X \subseteq \mathbb{R}$ is *quasi-concave* in x if the level sets, $S_\alpha = \{x : f(x) \geq \alpha\}$, are convex for all $\alpha \in \mathbb{R}$. The following definition by Jensen (2018) introduces the notion of *quasi-concave differences.*

Definition 2.1. (Quasi-Concave Differences). *The function $u : X \times T \mapsto \mathbb{R}$ is said to exhibit quasi-concave differences if for all $\delta > 0$ in a neighbourhood of 0, $u(x,t) - u(x-\delta,t)$ is quasi-concave in (x,t).*

An intuitive understanding of a function $u(x,t)$ that satisfies the quasi-concave differences property is that the influence of the decision variable, x, on the function u, reduces as the parameter t increases. For thrice differentiable functions, we refer the reader to Lemma 3 in Jensen (2018) which provides a condition on the derivatives that characterizes quasi-concave differences. Let $g(t)$ denote the greatest selection amongst the set of maximizers, $G(t)$, i.e., $g(t) = \sup\ G(t)$.

Theorem 2.2. *Let T be a convex subset of a real vector space and $X \subseteq \mathbb{R}$ be a convex subset of reals. Then, if $u(x,t) : X \times T \mapsto \mathbb{R}$ exhibits quasi-concave differences, $g : T \mapsto \mathbb{R}$ is concave.*

The above theorem follows directly from Jensen (2018) who proves a more general result. However, for our purposes, it is sufficient to restrict our attention to the greatest maximizer, $g(t)$, a single-dimensional real decision variable, x, and a constraint set, X, that is invariant with respect to the parameter t. In the appendix, for the sake of completeness, we provide a proof of Theorem 2.2 drawing upon the results of Jensen (2018). The above result is reminiscent of Topkis' (1978) theorem which demonstrates monotonicity of the optimizer subject to the objective function satisfying the closely related increasing differences propert, where $u(x,t)$ is said to possess the increasing differences property if for all $\delta > 0$ in a neighbourhood of 0, $u(x,t) - u(x-\delta,t)$ is increasing in t (Topkis 1978). Indeed, the main achievement of Jensen (2018) can be viewed as a second order extension of Topkis' theorem.

We now consider a collection of non-cooperative games, $\Gamma(t) = (N, X, \{u_i(\cdot,t) : i \in N\})$, that are parametrized by $t \in T$, where N denotes the set of all players, X is a compact and convex set of action vectors, and $u_i(x,t)$ corresponds to a continuous payoff function for player i given the action vector $x \in X$. For player $i \in N$, let $X_i \subset \mathbb{R}$ denote its own action set, and X_{-i} correspond to the action set for the rest of the players in $N \backslash \{i\}$. $\Gamma(t)$ is said to be a *supermodular game* if for each player $i \in N$, X_i is a compact subset of $\mathbb{R}$, and $u_i(x_i, x_{-i}, t)$ has increasing differences in (x_i, x_{-i}). These requirements imply that the action of a player is complementary with the actions of other players (Topkis 1998). The monotonicity of the equilibrium actions for the game $\Gamma(t)$ in t does not immediately follow from Topkis' (1978) results on the monotonicity of optima. However, Milgrom and Roberts (1990) employ Topkis' theorem alongside fixed-point arguments to develop conditions on the parametrized space of games such that the extremal equilibria of $\Gamma(t)$ are monotonic in t. We now provide an analogous result characterizing sufficient conditions for the greatest equilibrium of $\Gamma(t)$ to be concave in $t \in T$.

For parameter value $t \in T$, let $\tilde{x}(t) = \{\tilde{x}_i(t) : i \in N\}$ denote the greatest equilibrium action vector of $\Gamma(t)$. Following Definition 1, $u_i(x_i, x_{-i}, t)$ satisfies the quasi-concave differences property if for all $\delta > 0$ in the neighbourhood of 0, $u_i(x_i, x_{-i}, t) - u_i(x_i - \delta, x_{-i}, t)$ is quasi-concave in (x_i, x_{-i}, t).

Theorem 2.3. *Suppose that* $\Gamma(t) = (N, X, \{u_i(\cdot, t) : i \in N\})$ *is a collection of supermodular games parametrized by* $t \in T$ *where* T *is a convex subset of a real vector space. Further, for each player* $i \in N$*, suppose that* $u_i(x_i, x_{-i}, t)$ *satisfies the quasi-concave differences property. Assume that all equilibria of* $\Gamma(t)$ *are interior for all* $t \in T$*. Then, the greatest equilibrium action vector of* $\Gamma(t)$*,* $\tilde{x}(t)$*, is concave in* $t \in T$*.*

The above theorem states that for parametrized supermodular games that additionally satisfy the quasi-concave differences property, the greatest equilibrium action vector is concave in the parameter. Theorem 2.3, much like its counterpart for optimization problems, Theorem 2.2 due to Jensen (2018), is of independent interest for economic modelling applications and constitutes an important methodological contribution of this essay.

2.4.2 Shapley Allocation and Abatement Incentives

Let $\mathcal{P}_i$ denote the set of processes in the supply chain whose pollution can be influenced by firm i via the exertion of costly efforts. That is, process $j \in \mathcal{P}_i$ if and only if $b_{i,j} = 1$. In the first-stage of our model, we allow the firms to exert costly pollution abatement efforts so as to jointly reduce pollution in the supply chain. Formally, each firm i can introduce emission reduction efforts, $e_{ij} \in [0, 1]$, towards process $j \in M$. For clarity, the efforts, e_{ij}, could also correspond to indirect efforts and actions by firm i such as component design or packaging decisions which affect the direct emissions of other firms in the supply chain.

In contrast with the implicit treatment in §2.3 of the footprint of a process j, f_j, as a constant scalar input, in this section, f_j is considered to be a symmetric differentiable decreasing function of the emission reduction efforts, $f_j(\{e_{ij} : i \in N^j\}) = f_j(\boldsymbol{e_j})$. We assume that $f_j(\boldsymbol{e_j})$ is submodular in $\boldsymbol{e_j}$, that is, for firms $i, k \in N^j$, $\partial^2 f_j / \partial e_{ij} \partial e_{kj} \leq 0$. This reflects the complementary nature of emission reduction efforts exerted by firms in the supply chain. In addition, we assume that the first partial derivatives, $\partial f_j / \partial e_{ij}$, are convex in $\boldsymbol{e_j}$ for $i \in N^j$. The abatement cost incurred by a firm i towards exerting the effort, e_{ij}, $a_{ij}(e_{ij}) : [0, 1] \to [0, A]$ is also assumed to be strictly increasing, convex and with a non-negative third derivative, that is, $\partial a_{ij} / \partial e_{ij}$ is convex. The commonly assumed model of pollution abatement in the literature is of linear emission reduction with quadratic or cubic abatement costs (e.g., see Subramanian et al. 2007, and Parry and Toman 2002). We employ such a cubic abatement cost model in our numerical analysis in §2.6.3, and it is easily seen that these models satisfy all our assumptions.

As noted by Caro et al. (2013), linear sharing rules are the only type of allocation rules observed in practice and, moreover, non-linear differentiable rules could be replaced by linear sharing rules which would lead to the same outcome in the decentralized pollution reduction game (Bhattacharya and Lafontaine 1995). Therefore, we limit our attention in the second-stage to only linear allocation rules, $\phi = \{\lambda_{ij} : i \in N, j \in M\}$, that are footprint balanced, given by $\sum_{i \in N^j} \lambda_{ij} f_j = f_j$ and $\lambda_{ij} \geq 0$, for all processes j. In a decentralized supply chain, given the linear allocation rule ϕ, the first-stage emission reduction efforts exerted arise as an equilibrium of a non-cooperative game, $\mathcal{G}(\phi)$, with each player optimizing its own payoff function as follows, thereby ensuring incentive compatibility,

$$\{e^{\phi}_{ij} : j \in \mathcal{P}_i\} = \arg\min_{e_{ij}} \sum_{j \in \mathcal{P}_i} a_{ij}(e_{ij}) + \sum_{j \in \mathcal{P}_i} p^S \lambda_{ij} f_j(\boldsymbol{e_j}). \tag{2.5}$$

The social first-best pollution emissions value for the supply chain, $f^* = \sum_{j \in M} f_j(\boldsymbol{e^*_j})$, is obtained by solving the following optimization problem[15],

$$\boldsymbol{e}^* = \arg\min_{\boldsymbol{e}} \sum_{i \in N,\ j \in \mathcal{P}_i} a_{ij}(e_{ij}) + \sum_{j \in M} p^S f_j(\boldsymbol{e_j}). \tag{2.6}$$

Given the linear allocation rule ϕ, let $f^{\phi} = \sum_{j \in M} f_j(\boldsymbol{e^{\phi}_j})$ be the supply chain emission supported by the greatest equilibrium of the decentralized game.[16] The following proposition follows immediately from Proposition 2 of Caro et al. (2013) and demonstrates that in supply chains with joint production of pollution, footprint balanced emission sharing rules cannot achieve first-best emission reduction efforts in the decentralized game, that is, $f^{\phi} > f^*$.

Proposition 2.2. *For supply chains with joint production of pollution, that is, if there exists $j \in M$ such that $|N^j| > 1$, then, for all linear allocation rules ϕ, $f^{\phi} > f^*$.*

We therefore next address the question of identifying a unique *best* allocation mechanism, in terms of incentivizing emission reduction efforts, amongst the class of linear sharing rules which are footprint balanced. Since the pollution abatement technologies available to a firm and the corresponding cost functions, a_{ij}, are typically private information[17], the metric we adopt to evaluate a footprint-balanced allocation is its worst-case performance over all possible private abatement cost functions.

Definition 2.2. (Loss of Efficiency and Worst-Case Loss of Efficiency).
i. Loss of efficiency due to a sharing rule ϕ with a collective cost vector $\boldsymbol{a}$ is given by $\delta(\phi, \boldsymbol{a}) = f^{\phi} - f^* > 0$.
ii. The worst-case loss of efficiency is defined as $\Delta(\phi) = \max_{\boldsymbol{a} \in \mathcal{A}} \delta(\phi, \boldsymbol{a})$ for all $i \in N$, $j \in \mathcal{P}_i$, where $\mathcal{A}$ is the space of functions satisfying the abatement cost assumptions.

[15] As in Caro et al., (2013), we assume that abatement efforts, though costly, don't affect the firms' revenues from their core operations.

[16] If there are multiple equilibria, we take the one with the greatest efforts, i.e., the one minimizing the total supply chain emissions.

[17] See, e.g., Malueg and Yates (2009), Ross (1999).

The parametrized first-stage non-cooperative game, $\mathcal{G}(\phi)$, can be decomposed into $|M|$ supermodular games. We then apply the results of §2.4.1 to prove that the equilibrium efforts $\boldsymbol{e}^{\phi}$ are concave in ϕ. We prove these results in Lemma A.2 in Appendix A. This allows us to derive the following central result which identifies the Shapley allocation as a footprint-balanced linear sharing rule that minimizes the worst-case loss of efficiency.

Theorem 2.4. *For every linear allocation rule ϕ that is different from the Shapley allocation, Φ, $\Delta(\phi) \geq \Delta(\Phi)$.*

In the absence of the tools developed in §2.4.1, the second-order comparative statics needed to obtain the above theorem can only be performed by invoking the implicit function theorem twice over. As Jensen (2018) notes, this in turn will imply that "a host of unnecessary technical assumptions must be imposed – so even when the implicit function theorem provides sufficient conditions for concavity, these will not be the most general conditions". Such technical assumptions made to simplify the analysis shall render challenging the identification of the most general conditions that drive the result. Indeed, in the appendix we provide an alternate proof of Theorem 2.4 that solely relies on the implicit function theorem and therefore needs to employ additional restrictive separability assumptions.

We further point out that the symmetry of the Shapley allocation, as embodied by the Shapley's symmetry axiom (Shapley 1953), is not the driver of Theorem 2.4, since there are other allocation mechanisms that satisfy this symmetry axiom. Indeed, if the loss of efficiency were to be measured with respect to the total social cost, instead of the socially optimal supply chain emission level, then the worst-case loss of efficiency may no longer be minimized by the Shapley allocation.

Finally, we demonstrate in Theorem 2.5 below that, for the Shapley allocation rule, Φ, the gap $\delta(\Phi, \boldsymbol{a})$, between the supply chain emissions supported by the decentralized equilibrium, f^{Φ}, and the social first-best supply chain emissions, f^*, is bounded.

Theorem 2.5. *Consider a supply chain that employs the Shapley allocation rule, Φ, as the emission apportionment mechanism. Let f^0 denote the baseline emissions of the supply chain, that is, when firms do not exert emission abatement efforts. Then,*

$$\frac{\delta(\Phi, \boldsymbol{a})}{f^0 - f^*} = \frac{f^{\Phi} - f^*}{f^0 - f^*} \leq 1 - \frac{1}{\max\limits_{j \in M} |N^j|}$$

Theorem 2.5 bounds the gap, $\delta(\Phi, \boldsymbol{a})$, in terms of the extent of joint production of pollution in the supply chain. Trivially, if there is no joint production of pollution in the supply chain, i.e., for each process in the supply chain, there exists a unique firm that can influence its emissions, then the Shapley rule coincides with the total producer responsibility rule, and achieves full efficiency. That is, $\delta(\Phi, \boldsymbol{a}) = 0$. Further, in §2.6, we perform a numerical comparative statics analysis and demonstrate that the efficiency gap, $\delta(\Phi, \boldsymbol{a})$, is concave increasing in the prevailing carbon price p^S. Additional related numerical illustrations are also provided in §2.6.

Remark 2.2. *As previously mentioned in Footnote 15, following Caro et al. (2013), we assume that the revenue from core operations of the supply chain is unaffected. Then, supply chain profits are maximized when the total carbon penalty paid by the supply chain is minimized. Therefore, it follows from Theorem 2.4 that the Shapley allocation rule minimizes the carbon penalty paid by the supply chain, and equivalently maximizes supply chain profits, in a worst-case sense. Similarly, the bounds obtained in Theorem 2.5 also translate into bounds on the decentralized supply chain profits in relation to the first-best supply chain profits.*

2.5. Properties of the Shapley Allocation

In this section, we reveal that the Shapley allocation satisfies some additional properties that are contextually desirable from welfare and implementation perspectives. In fact, we show that it can be uniquely characterized by these properties, which provides a complementary approach to the problem of allocating emissions responsibility in a supply chain. Axiomatizations characterize a proposed solution mechanism on the basis of a certain set of properties and, as such, clarify the domain of applicability, and the strengths and limitations of the proposed solution concepts. To the extent that these properties are viewed as desirable, they make a more compelling case for the adoption of the proposed mechanism in the particular context. Axiomatic characterizations, such as Shapley's (1953) original characterization of the Shapley value, have played a key role in the development of cooperative games solution concepts in the game-theoretic literature. In related contexts, such as airport games and highway games, other axiomatizations of the Shapley value were developed, e.g., by Dubey (1982), Sudhölter and Zarzuelo (2017) and Rosenthal (2017).

First, recall that $f = [f_1, f_2, \ldots, f_m]$ denotes the total supply chain carbon footprint vector consisting of the pollution of all processes in the supply chain, and $\mathcal{P}_i$ denotes the set of processes that can be influenced by actions of firm i, i.e., $j \in \mathcal{P}_i$ iff $b_{i,j} = 1$. Further, let $\tilde{\mathcal{P}}_i$ denote the set of processes with non-zero pollution that i is responsible for. That is, $j \in \tilde{\mathcal{P}}_i$, iff $b_{i,j} = 1$ and $f_j > 0$. We recall that a pollution allocation rule ϕ is a function, $\phi(\mathbf{B}, f)$, which allocates to each firm, i, its responsibility, $\phi_i = \phi_i(\mathbf{B}, f)$, towards the total pollution such that $\sum_{i=1}^{n} \phi_i = \sum_{j=1}^{m} f_j$. We now consider certain intuitive properties which could naturally be expected from a pollution allocation rule. We also discuss their relevance in terms of the supply chain welfare generated by the allocation rule and its implementation.

No Free Riding: For any firm i and footprints $f' \geq f$, such that $f'_j = f_j$ for all processes j for which $b_{i,j} = 1$, $\phi_i(f') = \phi_i(f)$.

The *no free riding* property requires that if the total pollution increases, but for some firm, the pollution of the processes it is responsible for are unchanged, then the firm's allocation remains the same. In other words, an increase in pollution allocation for a firm is justifiable only if the pollution of the processes it has influence over increases. Equivalently, it also prevents *free-riding* of firm i on pollution abatement improvements by other firms on processes firm i is not responsible for. Lange (2006) also discusses the negative effects of free-riding and notes that preventing it improves the chances of cooperation in environmental agreements. Further, and most importantly, it can be easily seen that an allocation rule which does not satisfy the *no free riding* property can be modified into an allocation rule that offers the same emission reduction incentives to the firms in the supply chain at a strictly lower supply chain cost. Therefore, the supply chain welfare associated with a pollution allocation rule violating the *no free riding* property can always be improved upon.

Process history independence: Let $f' \geq f$ and $\tilde{f}' \geq \tilde{f}$ be footprints such that $f'_j = f_j$ and $\tilde{f}'_j = \tilde{f}_j$ for all processes $j \in M \backslash \{k\}$, $f'_k = \tilde{f}'_k$ and $f_k = \tilde{f}_k$. Then, for any firm i, $\phi_i(f') - \phi_i(f) = \phi_i(\tilde{f}') - \phi_i(\tilde{f})$.

Process history independence states that the change in responsibilities of the firms due to a change in pollution of any process is independent of the pollution levels of other processes. Process history independence emphasizes the ease of interpretation of an allocation rule. It implies that firms can find out the effect of an increase or decrease in the pollution level of a process independently of the pollution levels of other processes. Thus, it enhances the transparency of the effects of investment in pollution abatement technologies on the attributed emission responsibility. Further, and importantly, in a supply chain that is operating across multiple time-periods, an allocation mechanism which is not process history independent would incentivize firms to engage in manipulating or delaying the adoption of cleaner technologies in their processes. Thus, process history independence also ensures that the firms do not engage in strategic gaming of technology adoption decisions.

Disaggregation Invariance: Consider a supply chain with n firms, set of processes M, and a corresponding responsibility matrix $\mathbf{B}$. Suppose firm i chooses to disaggregate and represent itself as firms i_1 and i_2, such that $\mathcal{P}_{i_1} \cup \mathcal{P}_{i_2} = \mathcal{P}_i$ and $\mathcal{P}_{i_1} \cap \mathcal{P}_{i_2} = \emptyset$. The disaggregated supply chain now has $n+1$ firms, an identical set of processes M, and a corresponding responsibility matrix $\mathbf{B}'$, with $n+1$ rows, wherein row b_i, corresponding to row i in $\mathbf{B}$ has been replaced with rows $b^{'}_{i_1}$ and $b^{'}_{i_2}$ in $\mathbf{B}'$. Then, ϕ is said to be *disaggregation invariant* if for a firm $j \neq i$, $\phi_j(\mathbf{B}, f) = \phi_j(\mathbf{B}', f)$, and $\phi_{i_1}(\mathbf{B}', f) + \phi_{i_2}(\mathbf{B}', f) = \phi_i(\mathbf{B}, f)$.

Invariance of a pollution responsibility allocation to disaggregation of the supply chain is discussed by Lenzen et al. (2007) and also by Rodrigues and Domingos (2008). They argue that pollution responsibility allocations to firms should not change when a manufacturer, instead of selling directly, decides to disaggregate and sell via a distributor who creates no additional pollution. A pollution allocation rule that is not invariant under disaggregation would provide incentives for firms to resort to manipulation by de-merging while reporting emissions. Therefore, disaggregation invariance ensures a form of strategy-proofness of the allocation mechanism and assumes significance from an implementation perspective.

It is easy to show that the Shapley allocation, Φ, satisfies all the above properties. In fact, coupled with the natural *firm equivalence* property, which requires that two firms that are responsible for an identical set of polluting processes receive identical allocations,[18] and *firm nullity*, which states that a firm which is not responsible for any polluting process be allocated zero responsibility, we derive a unique characterization of the Shapley allocation provided in Theorem 2.6. Firm equivalence is a fundamental equity principle that enhances the acceptability of a pollution responsibility allocation mechanism.

Theorem 2.6. *The Shapley allocation, Φ, is the unique footprint balanced pollution allocation rule which is uniquely characterized by each of the following sets of independent properties:*
i. Process history independence, firm equivalence, and firm nullity.
ii. Disaggregation invariance, firm equivalence, and no free riding.

Finally, we note that a similar axiomatic approach in the context of environmental responsibilities is adopted by Rodrigues et al. (2006), who consider an input-output framework and impose six properties to derive a unique indicator of environmental responsibility. More recently, Kander et al. (2015) and Domingos et al. (2016) pursue this line of inquiry to allocate responsibilities to countries towards emissions arising from global trade.

2.6. Case Study – Walmart's Jeans Supply Chains

There are a variety of reasons for firms to be concerned with GHG emissions arising from their supply chains. While the financial impact of emission taxes in an increasing number of regions might be a reason, it has also been established that consumers do value the environmental sustainability of brands (Luchs and Kumar 2015; Nielsen 2018). Since emissions occur throughout the supply chain, it can be useful for leaders to account for the emissions from their supply chain members and identify opportunities for joint reduction of emissions. As elaborated in §2.1, Walmart is one of the companies that has embraced its responsibility to protect the environment and reduce emissions in its vast supply chain. Since their own operations account for roughly only 10% of their total supply chain GHG emissions, Walmart

[18] We note that firm equivalence is a weaker requirement than the classical axiom of symmetry in the original axiomatic characterization of the Shapley value.

has acknowledged the need to engage with their suppliers to realize a significant impact. For the purpose of this analysis, we focus on its apparels, and specifically, on its jeans brands and their supply chains.

Walmart offers a wide variety of jeans brands ranging across Levi Strauss & Co. (LS & Co.), Jordache, Lee, Wrangler, Democracy, Nautica, Gloria Vanderbilt and so on. We find considerable variation in the extent of sustainability initiatives undertaken by the brands. For instance, we were unable to find any public disclosure of information by Democracy and Nautica on their environmental performance. This does not necessarily imply that these companies are not working with their supply chain members towards reducing their emissions, however, we do note that environmentally-conscious companies typically opt to share their efforts and initiatives with the public. In that regard, we note that some consumers group are recommending "no buy" for Nautica's products in view of the lack of transparency of their sustainability initiatives.[19]

Across the various jeans brands, LS & Co. appears to be the most concerned with their overall environmental impacts engaging in sustainability efforts on several fronts. In this case study, we focus on two of Walmarts immediate suppliers, LS & Co. and Nautica. Based on the efforts undertaken by LS & Co. to reduce its supply chain emissions, we illustrate how Walmart can identify and assign indirect responsibilities to members in the Nautica supply chain. We then analyze the incentives and supply chain emission reductions achieved by the Shapley mechanism.

2.6.1 Levi Strauss' & Co.'s Environmental Initiatives

According to their 2018 Carbon Disclosure Project report[20], LS & Co. is engaged with its suppliers on different levels in efforts to reduce supply chain emissions. LS & Co. estimates that 99% of their total GHG emissions come from Scope 3 categories, and intends to work closely with their suppliers to establish targets for emission reductions and share practices around energy efficiency. In 2017, they engaged about 37% of their suppliers, focusing on those supplying a high volume of products and with significant potential for improvement opportunities. They collect suppliers' energy use and GHG emissions data annually (through the Sustainable Apparel Coalition's Higg Facility Environmental Module), and use this data for calculation of their Scope 3 emissions and to evaluate suppliers' engagement strategy. LS & Co. has committed to reduce their Scope 1 and Scope 2 emissions by 90%, and to reduce 40% of the emissions across their supply chain by 2025 from a 2016 baseline. We now describe some of their initiatives in greater detail.

Material Acquisition. Agricultural emissions from cotton farming is intimately linked

[19]See, for example, https://rankabrand.org/casual-clothing/Nautica/detailed-report

[20]https://www.levistrauss.com/wp-content/uploads/2018/03/Levi-Strauss-Annual-Report-2017.pdf

with water usage, and contributes substantially to the environmental footprint of LS & Co. They found that nearly 70% of water withdrawal occurs in the fiber phase (e.g., cotton growing) while 6% occurs in the fabric production phase (manufacturing). As a result, they are engaging with cotton farmers through participation in the Better Cotton Initiative (BCI), an organization that trains farmers to adopt cotton production practices which use less water, and which also yields as a result other ancillary benefits of reducing pesticide and fertilizer usage, preserving biodiversity, and improving soil health and labor standards. BCI farmers use up to 18% less water than non-BCI farmers in comparable locations. LS & Co. is also exploring innovative approaches to use recycled cotton, as they estimate that jeans manufactured with at least 15% recycled cotton saves as much water as that consumed in the entire manufacturing process. In 2017, LS & Co. sourced 34% of their total cotton (90% of their products are cotton-based) through BCI, with the goal of using 100% sustainable cotton through sources such as BCI by 2020. LS & Co. estimates costs invested in the Better Cotton Initiative at around $85,000.

MANUFACTURING. LS & Co. has begun working with some manufacturers to implement their recycle and reuse standards, which outline how garment facilities can safely implement processes and equipment within their facilities without compromising product quality and safety. LS & Co. has partnered with the Natural Resource Defense Council (NRDC) on the Clean by Design Program, an initiative to reduce the environmental impact of textile mills in China. Six textile mills in China that supply fabric to LS & Co. participated in this program, achieving a total savings of 57,465 tons of steam and 2.62 million kWh/year over a five-year period.

LS & Co. is collaborating with the International Finance Corporation (IFC), the financing arm of the World Bank, to provide access to advisory services and low-cost financing to suppliers who wish to invest in reducing their energy, emissions, and water footprint, but need technical support or capital to do it. In 2017, LS & Co. started a pilot program with the IFC's Partnership for Cleaner Textile (PaCT) program, whereby LS & Co. is working with six of their manufacturers and is covering their cost to undergo a renewable energy assessment. If the on-site renewable investment is feasible, LS & Co. collaborates with IFC on a financing model which provides access to capital for sustainability investments. In less then a year, participating suppliers reduced their GHG emissions by an average of 13% and their energy use by an average of 22%. LS & Co. plans to expand the PaCT program to more factories and fabric mills, which have a larger carbon footprint than their current manufacturing facilities. In 2018, they made a plan to include mills in India, Pakistan, and Mexico, with the goal of engaging all wet processing suppliers globally within the next five years. LS & Co. estimate that they will invest around $2,400,000 in more efficient production processes at key supplier locations through the PaCT program in period 2018-2023.

Evidently, as can be seen from the above discussion, LS & Co. is not only making efforts to improve their own carbon footprint. Indeed, they are also actively engaging their suppliers to help them improve their environmental performance, which is in line with Walmart's vision of reducing emissions across their entire supply chain.

2.6.2 Walmart-Nautica Supply Chain

As discussed above, it appears that there are several suppliers of Walmart that are not sufficiently concerned with either their own sustainability or that of their respective supply chains. A possible way to incentivize them to do so, as modelled in this essay, is to hold them jointly responsible for emissions of their upstream partners whose emissions they can influence. Given the successful efforts by LS & Co. to address sustainability issues in its supply chain, it is reasonable to assume that Walmart could expect its other major suppliers to follow suit. Huang et al. (2019), in fact, find that such environmental supply chain governance involving monitoring and knowledge sharing across suppliers can lead to significant emissions reductions for firms as well as suppliers. Therefore, if Walmart's immediate supplier, say, Nautica, is held jointly responsible for the emissions of some of its supply chain members, then Nautica would be incentivized to work with its suppliers to help them reduce their footprint. For instance, similarly to LS & Co., Nautica can help provide funding or expertise assistance to their mills that want to reduce their energy emissions. It is in this context that the allocation scheme proposed in this work can be employed as a transparent mechanism that can suitably incentivize firms to reduce their joint emissions.

LS & Co. created a detailed LCA report (LS & Co. 2015) for the supply chain of Levi's 501®jeans for the production year 2012. We present a summary of their results in Table 2.1 and assume that the emission values are appropriate representative estimates for the emissions that a pair of Nautica jeans generates throughout its different life cycle stages. Indeed, to confirm the robustness of the emissions data, we further checked an apparel industry-wide study, Zeller et al. (2017), which included 159 life cycle inventories in compliance with ISO 14044. While there was a minor discrepancy between Levi's and Zeller et al.'s (2017) estimates since the latter included accessories such as leather patches while the former did not, overall, the data is in line with the apparel industry-wide, category-specific study of Zeller et al. (2017).

From Table 2.1, we observe that across the entire life cycle, from material acquisition to end of life, the manufacturing and consumer use stages each contributes 9 kg CO_2E and 12.5 kg CO_2E of the total emissions (33.4 kg CO_2E). In comparison, packaging and end of life account for a much smaller fraction of the emissions respectively.

	Raw Materials	Manufacturing	Assembly	Packaging	Transportation	Consumer Use	End of Life	Total
Stage	1	2	3	4	5	6	7	NA
Joint Responsibility	1, 3	2, 3	3	4	5	NA	NA	NA
Emissions (kg CO_2E)	2.9	9	2.6	1.7	3.8	12.5	0.9	33.4
Percentage ‡	14.5%	45.0%	13.0%	8.5%	19.0%	NA	NA	100%

Table 2.1: GHG emissions through the cycle of a pair of jeans.
‡Percentage is calculated with respect to the scope including stages 1 to 5 only.

Naturally, in practice, the processes and the resulting emissions may need to be allocated at a more granular level than what is represented in Table 2.1. That is, to implement the carbon emissions allocation scheme in practice, it may be necessary to break down the various processes to finer sub-processes, and allocate appropriate pollution responsibilities for the sub-processes using the methodology developed above.

Now, for the purpose of our subsequent analysis, we restrict the scope of the supply chain to Stages 1 to 5. This linear supply chain is responsible for a total of 20 kg CO_2E of emissions. We also note that Nautica has direct control over the assembly stages. In line with the efforts undertaken by LS & Co., suppose that Walmart also holds Nautica jointly responsible for emissions from material acquisition and manufacturing. Our objective is to apply the emissions allocation rule developed in this essay to incentivize the firms to exert joint emission reduction efforts across the supply chain.

2.6.3 Numerical Analysis

For the five-stage Nautica supply chain described above, given the joint responsibilities identified from the knowledge of successful initiatives by LS & Co., it follows from Theorem 2.1 that the Shapley allocation rule will split in half the emissions of Stages 1 and 2 between the upstream supply chain member and Nautica. Further, the emissions of the rest of the stages will be solely attributed to the corresponding supply chain firm by the Shapley rule. We consider the supply chain to be operating under a uniform carbon price of $p^S = 3¢/\text{kgCO}_2\text{E}$. This is reflective of carbon tax rates in Canada and is close to the estimated social cost of carbon in 2015 (Nordhaus 2015).

Material Acquisition. We consider a commonly assumed model of joint pollution abatement in the literature, of a linear and separable emission reduction with cubic abatement costs, to analyze the abatement incentives offered by the Shapley allocation. We note that our model satisfies the assumptions of §2.4.2 as well as the more restrictive assumptions on the abatement costs discussed in the appendix. Suppose that the emissions, f_1, at Stage 1 of the supply chain per unit of product (i.e., for each pair of jeans), is given by $f_1(e_{11}, e_{31}) = f_1^0 - \alpha_1(e_{11} + e_{31})$, where $f_1^0 = 2.9$ denotes the baseline emissions of Stage 1 (refer to Table 2.1) and we assume $\alpha_1 = 1$. The assumption of perfect substitutability of efforts by firms 1 and 3 is reflective of the substitutability of monetary investments in recycling. We also performed the numerical analysis with non-separable joint emission production functions and the results were qualitatively similar. The corresponding abatement costs are denoted by $a_{11}(e_{11}) = \beta_{11} e_{11}^h$ and $a_{31}(e_{31}) = \beta_{31} e_{31}^h$ with $h = 3$. The precise values of the cost parameters β_{11} and β_{31} are private information, as modelled in §2.4. For the purpose of our numerical analysis, we assume the supply chain leader's information about the distribution of these private cost parameters is that $\beta_{11}, \beta_{31} \in [10, 15]$.

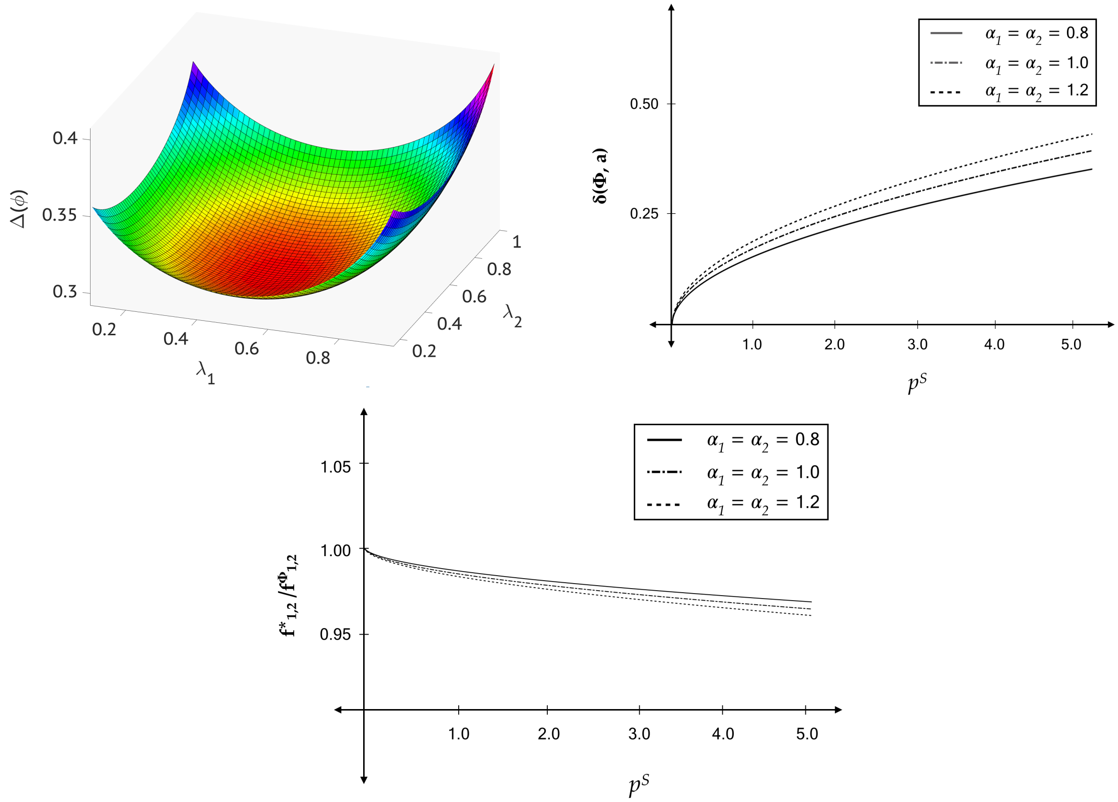


Figure 2.1: Worst-case loss of efficiency, $\Delta(\phi)$ (units: kgCO_2E), in the Nautica-Walmart supply chain is minimized at the Shapley allocation rule, Φ (left panel). The efficiency gap, $\delta(\Phi, \boldsymbol{a})$ (units: kgCO_2E), is concave increasing in the carbon price, p^S (units: ¢/kgCO_2E) (right panel). The ratio of first-best emissions to the emissions supported in equilibrium by the Shapley mechanism, $f^*_{1,2}/f^{\Phi}_{1,2}$, as a function of the carbon price, p^S (bottom panel).

Manufacturing. Suppose that the emissions, f_2, at Stage 2 of the supply chain for each pair of jeans, is given by $f_2(e_{22}, e_{32}) = f_2^0 - \alpha_2(e_{22} + e_{32})$, where $f_2^0 = 9$ denotes the baseline emissions of Stage 2 and assume $\alpha_2 = 1$. The corresponding abatement costs can be denoted by $a_{22}(e_{22}) = \beta_{22} e_{22}^h$ and $a_{32}(e_{32}) = \beta_{32} e_{32}^h$ with $h = 3$. As above, we also tested non-separable joint emission production functions and the results were qualitatively similar. We again note that the precise values of the cost parameters β_{22} and β_{32} are private information and, we assume the supply chain leader only knows that $\beta_{22}, \beta_{32} \in [30, 45]$.

Any linear allocation rule is uniquely parametrized[21] by the fraction of pollution at Stage 1, that firm 1 is allocated responsibility for, denoted by λ_1, and the fraction of pollution at Stage 2, that firm 2 is allocated responsibility for, denoted by λ_2. For all combinations of (λ_1, λ_2) such that $0 \leq \lambda_1, \lambda_2 \leq 1$ and a given realization of the cost parameters, the equilibrium joint efforts exerted by firms in the supply chain towards reducing their emissions can be computed from the equation (2.5). Then, the computation of the first-best reduction in emissions, given by (2.6), allows us to identify the worst-case loss of efficiency, $\Delta(\phi) = \max_{a_{ij} \in \mathcal{A}} \delta(\phi, \boldsymbol{a})$, where $\mathcal{A}$ is the space of possible realizations of the private cost functions. The left panel of Figure 2.1 is a surface plot of the worst-case loss of efficiency, $\Delta(\phi)$, over all possible linear allocation rules, ϕ, in the supply chain. It is seen that $\Delta(\phi)$ is minimized precisely at the Shapley allocation rule as predicted by Theorem 2.4. Further, we set $\beta_{11} = \beta_{31} = 10$ and $\beta_{22} = \beta_{32} = 30$, and in the right panel of Figure 2.1, we plot the loss in efficiency associated with the Shapley allocation mechanism, i.e., the efficiency gap $\delta(\Phi, \boldsymbol{a})$ as a function of the prevailing carbon price p^S. We observe that the efficiency gap is concave increasing in the carbon price p^S. In the bottom panel of Figure 2.1, we plot an alternate measure of the effectiveness of the allocation mechanism given by $f^*_{1,2}/f^{\Phi}_{1,2}$, where $f^*_{1,2}$ and $f^{\Phi}_{1,2}$ correspond to the combined emissions of the material acquisition and manufacturing stages of the supply chain under the first-best setting and under the Shapley mechanism, respectively. We focus on the first two processes because the first-best emissions and the emissions supported by the Shapley mechanism across the other three processes are identical. Finally, we note that when the carbon price $p^S = 3$¢/kgCO_2E, the emissions of the processes 1 and 2 in the first-best scenario correspond, respectively, to 2.2675 kgCO_2E and 8.6348 kgCO_2E as compared to the baseline emissions of 2.9 kgCO_2E and 9 kgCO_2E, respectively. The Shapley allocation mechanism results in emissions of 2.4527 kgCO_2E and 8.7418 kgCO_2E for the two processes. That is, $f^0_{1,2} = f^0_1 + f^0_2 = 11.9$ kgCO_2E, $f^{\Phi}_{1,2} = 11.1945$ kgCO_2E and $f^*_{1,2} = 10.9023$ kgCO_2E and therefore, the Shapley mechanism captures 70.7% of the emissions reduction from the baseline mechanism as compared to the first-best outcome.

2.7. Concluding Remarks

We provide in this essay a methodological contribution to aid in rationalizing CO_2 emissions in supply chains, which account for more than 20% of global GHG emissions. We consider supply chains with dominant leaders who are motivated to reduce pollution in their supply

[21] Without loss of generality, we implicitly assume that the allocation rules satisfy the "no-free riding" property.

chains, that either operate in an environment in which a carbon tax is in effect, or who implement an internal carbon-pricing system. We propose that the supply chain leaders can leverage their knowledge on the interrelated sources of pollution in their supply chains, and re-allocate emissions within the supply chain in a footprint-balanced manner. This is equivalent to redistributing the carbon tax burden across the supply chain, and is carried out by the supply chain leaders so as to incentivize firms to exert efforts to jointly reduce their "indirect" emissions. We formulate the re-apportionment problem as a cooperative game, referred to as the GREEN game, and propose the Shapley value of the GREEN game as a scheme to allocate responsibilities for total emissions in the supply chain. We show that the Shapley allocation incentivizes abatement efforts that are optimal, in a well-defined sense, when the abatement costs are private information. Finally, we provide a proof of concept by carrying out a case study of the Walmart-Nautica jeans supply chain wherein we contextualize our results.

In view of the reluctance of suppliers to share information about their GHG emissions (see, e.g., Jira and Toffel 2013), it is important to note that the Shapley value of the GREEN game is both transparent and fair. It is shown to possess some contextual desirable properties with implications for welfare and implementation. Methodologically, we also exemplify the utility of an axiomatic development to identify desirable cost sharing mechanisms in supply chains.

Future Work

We note that in our model, as in Caro et al. (2013), firms were assigned joint responsibilities for GHG emissions occuring at other firms in the supply chain exclusively for the reason that they can take action to reduce, perhaps at a cost, emissions at those firms. However, responsibilities could possibly stem from other considerations. For example, it may be desirable to hold energy producing firms indirectly responsible for the downstream pollution impact of their projects, or hold firms responsible for the direct emissions at their upstream suppliers, or require consumers to internalize the cost of the GHG pollution in the supply chains which are used to produce the products they consume.

Indeed, numerous countries use GHG accounting methodologies that make them responsible only for the emissions they create within their own borders. For instance, according to Porter (2013), about a fifth of China's emissions are for products consumed outside its borders, and while Europe emitted only 3.6 billion metric tons of CO_2 in 2011, 4.8 billion tons of CO_2 were created to make the products Europeans consumed in that year. Naturally, our approach, and in particular, the Shapley allocation, could be applied to inform the analysis and derive footprint-balanced emission responsibility allocation schemes in global supply chains or, in general, in instances where the assignment of pollution responsibilities stem from different reasons.

We also note that the problem of incentivizing firms to increase emission abatement efforts in supply chains can be studied in a variety of other related or more general settings. In this work, we assume a fixed supply chain structure and we do not model endogeneity of prices within the supply chain. Indeed, to better understand the performance of footprint-balanced emission allocation mechanisms, such as the Shapley allocation, it is important to find their effectiveness to reduce emissions in a more general setting that relaxes these assumptions. Extensions of our work could also incorporate stochasticity in emission output, or imperfect or partial monitoring, or repeated interactions among the firms in the supply chain. Finally, a key methodological contribution in this essay is Theorem 2.3, which provides conditions ensuring concavity of equilibrium actions in parametrized non-cooperative games, thereby generalizing the results of Milgrom and Roberts (1990). We anticipate the result to find several applications in disparate domains.

Chapter 3

Consistent Allocation of Emission Responsibility in Fossil Fuel Supply Chains

3.1. Introduction and Literature Review

With rising awareness on the global impacts of greenhouse gases, countries across the world are adopting strategies to curb and regulate their carbon emissions. Indeed, fossil fuel burning accounts for close to 75% of the increase in global CO_2 levels in the past 20 years (IPCC 2014), and while the share of renewable energy sources is growing, fossil fuels continue to dominate, contributing to approximately 65% of electricity generation and powering over 90% of transportation in the United States (EPA 2016).

In a globalized world, fossil fuel supply chains are increasingly complex and spread across several jurisdictions. Fossil fuels are often extracted, refined and ultimately burnt in different countries. Accounting and assigning responsibility for these emissions is an essential component of any integrated climate action program. Harrison (2015) notes that the United Nations' Framework Convention on Climate Change (UNFCCC) only assigns responsibility for emissions that occur within a country's borders. Thus, neither is an exporter of fossil fuels assigned any responsibility towards the inevitable emissions generated while they are burnt, nor is the importer assigned any responsibility towards the extraction emissions associated with the fossil fuel. Environmental NGOs and activists such as Monbiot (2015) also argue for abandoning a wholly consumption-focused approach and to move towards assigning responsibility to both the producers and consumers of fossil fuels.

Although a significant fraction of carbon emissions in the fossil fuel supply chain arises downstream during the consumption stage, the upstream stages of extraction and refining often contribute close to 20% of the total supply chain emissions (OSM 2019). Unconventional petroleum deposits such as the Canadian oil sands typically entail higher upstream emissions during the extraction, transportation of the denser bitumen through pipelines, and the refining stages (Charpentier et al. 2009). In most countries, only the direct emissions of firms have been regulated (Oh et al. 2015). However, acknowledging the necessity of assigning extended responsibility, the Canadian federal government announced on January 27, 2016 that the energy regulator of Canada, National Energy Board (NEB), would factor in upstream emissions during the environmental impact assessment stage for proposed energy projects (Canada 2016). Upstream emissions are defined as emissions associated with "all industrial activities from the point of resource extraction to the project under review" (Canada 2016). This could have significant implications for several pipeline projects across Canada that transport crude oil or refined products to refineries and shipping terminals. The upstream emissions attributable to a proposed project could be compared against a rejection threshold level of emissions whereby the regulator, NEB, sets a predetermined level of upstream emissions beyond which the project will be rejected or the regulator could instead require the firm to offset some or all of the associated upstream emissions (Schaufele 2016).

A rejection threshold policy or offset requirements that take into account all upstream emissions of an energy project would have to be calibrated, depending on the stage of the supply chain the project is situated at, otherwise it risks inducing distortionary effects by favouring upstream energy projects over more downstream ones. This is primarily a consequence of double counting by attributing to each entity in the supply chain all associated upstream emissions. Another drawback of such a double counting method is that with a carbon offset program, it opens up the possibility of multiple parties claiming an offset for the same reduction in carbon emissions as part of their mitigation efforts, damaging the credibility of carbon offsetting (Schneider et al. 2014).

Our central objective is to develop a consistent accounting and implementation mechanism to allocate responsibility for greenhouse gas emissions in fossil fuel supply chains that potentially span multiple legal jurisdictions, while avoiding double counting and remaining concordant with the principle of upstream emission responsibility. We adopt a cooperative-game theoretic model of a fossil fuel supply chain represented by a directed tree, in which the players (or nodes) correspond to the extractors, distributors, refineries and end-consumers, and propose the nucleolus of the associated cooperative game as a mechanism to attribute upstream emission responsibilities in fossil fuel supply chains. We further evaluate and justify our proposed allocation mechanism along five broad criteria that the Government of Canada (2005) has identified as yardsticks to assess environmental policy proposals: (i) environmental effectiveness, (ii) fiscal impact, (iii) economic efficiency, (iv) fairness, and (v) simplicity of administration.

Review of Related Literature

We draw upon and contribute to two main streams of literature: emissions accounting in supply chains, and the application of cooperative game theory in supply chain management. In the environmental literature, several methods to allocate shared emission responsibility have been proposed by, e.g., Gallego and Lenzen (2005) and Lenzen et al. (2007). Their non-game theoretic models share similarities with our approach, as will be further elaborated in the sequel. The problem of identifying emission responsibility sharing mechanisms has also received some attention in the supply chain literature in particular contexts and Sunar (2016) provides an overview of some existing research addressing these issues. Sunar and Plambeck (2016) evaluate different methods of allocating carbon emissions among co-products. Benjaafar et al. (2013) study simple supply chain settings and their extensions by incorporating carbon footprint considerations.

Caro et al. (2013) analyze general supply chains with joint production of GHG emissions wherein firms facing a carbon price can jointly affect emissions via costly abatement possibilities. They show that when a central planner allocates emission responsibilities to individual firms in the supply chain, and imposes a cost on them proportional to these responsibilities, then, emissions typically need to be over-allocated to induce socially optimal abatement effort levels, even if the carbon tax is the true social cost of carbon. However, as noted by Caro et al. (2013), regulators may be unlikely to implement mechanisms that double-count, and if double counting is to be avoided, "allocation rules that are complex, non-continuous, and likely to be seen as unfair" have to be implemented to induce socially optimal abatement effort levels.

Relatedly, Gopalakrishnan et al. (2018) also consider a general supply chain with joint production of GHG emissions, and employ a cooperative game theory approach to address the inverse question of identifying a footprint balanced emission allocation mechanism in this setting. Based on the capabilities of firms to abate indirect emissions in the supply chain, they formulate a cooperative game, refereed to as the GREEN game, and propose a specific allocation mechanism, the Shapley value of the GREEN game. The Shapley allocation is shown to incentivize suppliers to exert pollution abatement efforts that are worst-case socially optimal when the pollution abatement costs are private information. Similar to Gopalakrishnan et al. (2018), in this paper we also employ a cooperative game theory approach for the problem of emission allocation in fossil fuel supply chains. However, unlike Gopalakrishnan et al. (2018), our cooperative game model is not formulated on the basis of ability of firms to abate indirect emissions. Rather, it arises from entirely different considerations, that is, to model new Canadian regulations that mandate factoring in upstream emissions while considering the environmental impact of energy projects.

In operations management, cooperative game theory has been adopted to address problems of sharing the benefits of cooperation between independent entities. In this stream of work, various solution concepts are studied as potential mechanisms for sharing profits or cost savings from cooperation. For example, the core of a game is used in inventory sharing problems, see, e.g., Hartman et al. (2000), and Anupindi et al. (2001), the Shapley allocation is employed, for example, in transshipment games (see, e.g., Granot and Sošić 2003, and Sošić 2006), and to allocate the excess profits of inventory pooling (Kemahlioğlu-Ziya and Bartholdi 2011), and the nucleolus was studied in the context of allocating cost savings from sharing demand information in a three-level supply chain (Leng and Parlar 2009). Nagarajan and Sošić (2008) provide a comprehensive overview of applications of cooperative game theory in the supply chain management literature.

Our work is also related to a branch of the cooperative game-theoretic literature concerned with cost allocation problems on graphs, such as the minimum cost spanning tree (mcst) game, see, e.g., Granot and Huberman (1984). A special case of an mcst game is the tree game (Megiddo 1978, and Granot et al. 1996), and both models are extensions of the airport game, e.g., Littlechild (1974). In the three models, the players[1] are represented by nodes in a graph, the cost associated with the edges designate maintenance or construction costs, and the objective is to allocate the total cost of construction or maintenance of the network in a fair manner. As is the case in this paper, the fair allocation method studied in the above four papers is the nucleolus of the respective cooperative games. Our cooperative game model can also be shown to be a generalization of the airport game that is, however, distinct from the tree game model. Our algorithm to compute the nucleolus is distinct from those developed in Megiddo (1978) and Granot et al. (1996) for the tree game model. Moreover, in contrast with the above papers, we employ the non-cooperative game theory paradigm to further investigate implementation and stability properties of the nucleolus, as well as study its ability, in our context, to incentivize the adoption of abatement technologies in fossil fuel supply chains.

From a methodological perspective, we also contribute to the *Nash program*, a research agenda which seeks to provide a non-cooperative foundation for solution concepts of cooperative games. In particular, for recent implementations of the Shapley value, see, e.g., Ju and Wettstein (2009), and Albizuri et al. (2015), and for implementations of the nucleolus, see, e.g., Serrano (1995), Dagan et al. (1997), and Albizuri et al. (2017).

Plan of the Paper

In §3.2, we first develop a cooperative game model for the problem of allocating emission responsibility in fossil fuel supply chains while incorporating the principle of upstream emission responsibility. We then formulate the *regulator's problem* as an optimization model that

[1]In the airport game, the players correspond to landings by airplanes of differing sizes.

maximizes the incentives offered by an allocation mechanism to firms for adopting potentially available emission abatement technologies, subject to some natural constraints, including a consistency requirement that is important in the regulatory context of emissions allocation. In §3.3, we characterize (Theorem 3.1), in our setting, a commonly used cooperative game-theoretic solution concept, the nucleolus, demonstrate that it is a feasible solution to the regulator's problem (Theorem 3.2), and develop a quadratic time algorithm (Theorem 3.3) for its computation. §3.4 provides an implementation framework for the nucleolus. Specifically, we construct a novel sequential non-cooperative alliance formation game, governed by two simple policies, which is shown (Theorem 3.4) to induce profit maximizing firms to adopt the nucleolus allocation. Further, we prove therein (Theorem 3.5) that the nucleolus allocation is the unique strong Nash-stable allocation subject to the two policies. The self-implementing nature of the policy framework for the nucleolus, as well as its stability and consistency properties, make the nucleolus an attractive allocation scheme in fossil fuel supply chains that, e.g., span multiple legal jurisdictions. In §3.5, we establish certain desirable and insightful structural properties (Propositions 3.5 - 3.8) of the nucleolus mechanism. In §3.6, we provide (Theorem 3.6) lower-bound guarantees on the welfare gains it delivers to firms and the incentives it offers (Theorems 3.6 and 3.7) to adopt potentially available emission abatement technologies. We further compare (Theorem 3.8), using these criteria, the performance of the nucleolus mechanism relative to the Shapley mechanism and the socially optimal allocation rule for certain specific supply chain configurations. Finally, in §3.7, we focus our attention on a proposed energy project in Canada, the extension of the Trans Mountain pipeline from the oil sands of Alberta to the ports of British Columbia. We perform a well-to-wheel carbon footprinting analysis and evaluate the performance of the nucleolus allocation relative to other allocations in terms of the incentives it generates to adopt emission reducing technologies and the social welfare it delivers. This helps us contextualize our work, which, hopefully, will also serve as a useful case study for policy makers and NGOs in their evaluation of the environmental liability of similar energy projects in other regions.

3.2. Model Development

We first briefly present some basic definitions and concepts of solution in cooperative game theory that will guide our model development and analysis.

3.2.1 Preliminaries

A cost cooperative game is denoted by (N, c) where N is the set of players, and c is the characteristic cost function which assigns to each subset S of N, $c(S)$, the cost of coalition S, where $c(\phi) = 0$. The game (N, c) is said to be *monotone* if the characteristic function c is monotone, that is, $c(S) \leq c(T)$ for $S \subset T \subseteq N$, and if $c(S \cup \{i\}) - c(S) \geq c(T \cup \{i\}) - c(T)$ for all $S \subseteq T \subseteq N$ and $i \in N$, then (N, c) is said to be a *concave* game.

A cost allocation vector $x = (x_1, ..., x_n)$ which allocates to each player i a cost, x_i, is said to be a *preimputation* if $\sum\limits_{i \in N} x_i = c(N)$. It thus allocates the total cost of the grand coalition, N, among all the players. A preimputation x for which $x_i \leq c(\{i\})$, $i \in N$, is referred to as an *imputation*. The *core*, $\mathcal{C}(N, c)$, consists of all vectors $x = (x_1, x_2, \ldots, x_n)$ such that no subset of players, S, is allocated more than its associated cost, $c(S)$. That is, $\mathcal{C}(N, c) = \{x \in R^n : x(S) \leq c(S), \forall S \subset N, x(N) = c(N)\}$, where $x(S) \equiv \sum_{j \in S} x_j$. The core is thus the set of preimputations which are *individually rational* (i.e., $x_i \leq c(\{i\})$ for each i) and *coalitionally rational* (i.e., $x(S) \leq c(S)$ for each $S \subseteq N$). But the core could be empty, and even if non-empty, it usually does not consist of a single allocation. For monotone games with a non-empty core, it can easily be shown that the core vectors are non-negative. For concave games, the core is non-empty (Shapley 1971).

An important solution concept for cooperative games, introduced by Schmeidler (1969), is the nucleolus. Intuitively, the nucleolus is based on the principle of minimizing the maximum dissatisfaction over all possible coalitions in a lexicographic manner. Formally, let $e_S(x) = c(S) - x(S)$ denote the *excess* of coalition S with respect to the allocation x. The smaller the excess, the more dissatisfied the coalition S is with x. For each x, let $e(x) = (e_S(x))_{S \in 2^N \setminus \{N, \emptyset\}}$ in which the excesses are arranged in an increasing order. The nucleolus z is the unique imputation that lexicographically maximizes the excesses of all coalitions. That is, $e(z) \succ_l e(x)$ for all other imputations x, where $\succ_l$ denotes the lexicographic order. The nucleolus, by sequentially maximizing the welfare of the least well off coalitions, imports the Rawlsian notion of fairness to cooperative games.

The pre-kernel of (N, c), another solution concept for cooperative games, is based on bargaining power considerations. Introduced by Davis and Maschler (1965), it consists of all allocations $\{x \in \mathbb{R}^n : x(N) = c(N)$ and $s_{kl}(x) = s_{lk}(x)$, for all $k, l \in N, k \neq l\}$, where $s_{kl}(x) = min\{c(S) - x(S) : k \in S, l \notin S\}$ denotes the maximum surplus of player k in the absence of player l. The maximum surplus $s_{kl}(x)$ is an intuitive measure of the bargaining power of player k over player l with respect to x, and the pre-kernel balances the maximum surplus for each pair of players. In concave games, the pre-kernel consists of a unique point in the core and coincides with the nucleolus (Maschler et al. 1971), thus providing an alternate interpretation of the nucleolus for the class of concave games.

Despite the attractiveness of the nucleolus as a solution concept, its computation could be prohibitive. However, it can be efficiently computed in a variety of settings - including, for example, three-player cooperative games (Leng and Parlar 2010), airport games (Littlechild 1974), standard tree games (Meggido 1978 and Granot et al. 1996), and assignment games (Solymosi and Raghavan 1994). One of the contributions of this paper is the development of a quadratic time algorithm to compute the nucleolus of a cooperative game which models the allocation of upstream emission responsibilities in fossil fuel supply chains.

3.2.2 A Cooperative Game Model

We now introduce our cooperative game model that underpins the subsequent development of a mechanism to allocate upstream emission responsibilities in fossil fuel supply chains. We consider a supply chain enterprise, defined by $\mathcal{SC} = (V, E, a, N)$, where V and E are the vertex and edge sets, respectively, of the directed tree, T, with a root node denoted by 0. The vertex set, $V = N \cup \{0\}$, where N designates the set of all the firms in the supply chain enterprise and $n = |N|$ corresponds to the number of firms in the fossil fuel supply chain[2]. A firm (or project) i in the fossil fuel supply chain is associated with node i, $i \in N$, where node 1 represents the most downstream member of the supply chain, and we assume that a single arc emanating from node 1 enters node 0. Typically, node 1 could designate the end consumers or retailer in the fossil fuel supply chain. The leaf nodes represent the most upstream firms, typically extractors of fossil fuels, and the other nodes represent intermediate firms or distributors. Each edge e in E is associated with a process or an activity in the fossil fuel supply chain emitting a pollution, $a(e)$.

Following standard convention and Canadian guidelines (Canada 2016), the emissions, $a(e)$, associated with the activity corresponding to the arc e, can be estimated by firstly identifying the throughput and its constituent distinct components flowing through the fossil fuel supply chain under consideration. Then, summing over the throughput of each individual component, multiplied by its GHG emission factor, results with the activity's emissions. The computations we perform for the Trans Mountain Pipeline case study are provided in Appendix II and serve as an illustration of this step. However, since the emissions at each stage in the supply chain serve solely as inputs to our model, we refer the reader to communication by the Department of Environment and Climate Change (Canada 2016) for further details on the estimation methodology.

Let e_i denote the unique edge in T emanating from node i in the direction of the root node of T. Then, $a(e_i)$, the pollution associated with e_i, represents the pollution directly created by firm i. Aside from the direct responsibility for the pollution $a(e_i)$, the regulatory principle of assigning upstream emission responsibility implies that firm i is also indirectly responsible for emissions generated from all activities upstream to it. Accordingly, for each firm i, we denote by $\mathcal{U}_i$ the set of edges in the subtree of T rooted at node i, and including e_i. Therefore, firm i is responsible for the pollution associated with the set of edges in $\mathcal{U}_i$. Such an interpretation of $\mathcal{U}_i$ is in line with the principle that each firm be held indirectly responsible

[2]We note that the root node 0 is a pseudo-node that does not correspond to any entity in the supply chain.

for the pollution arising from all upstream activities from the point of resource extraction up to and including the direct operations of the firm or project under consideration. We then define the *Upstream Responsibility* cooperative game, (N, c), induced by an $\mathcal{SC}$ enterprise, whereby for each S in N, $c(S) = a(\cup_{i \in S} \mathcal{U}_i)$. The total pollution emitted by the supply chain is $c(N) = \sum_{e \in E} a(e)$, and we seek to identify an apportionment of responsibilities, $\{x_i\}_{i \in N}$, of the total emissions among the firms, such that,

$$\sum_{i \in N} x_i = c(N). \tag{3.1}$$

Further, for $i, j \in N$, let $i \succ j$ denote that a firm i is downstream to another firm j. Then, an interpretation of the upstream responsibility principle implies that, since all the supply chain processes upstream to firm j are also upstream to firm i,

$$x_i \geq x_j, \quad \forall\, i \succ j. \tag{3.2}$$

Therefore, allocation mechanisms, $\{x_i\}_{i \in N}$, that satisfy the above property are said to be *concordant* with respect to the principle of upstream responsibility.

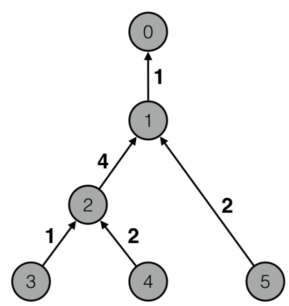


Figure 3.1: Illustrating the Upstream Responsibility game model for a simple fossil fuel supply chain.

Example 3.1. *As an illustrative example to clarify the above discussion, consider* $N = \{1, 2, 3, 4, 5\}$ *as the set of firms in the fossil fuel supply chain depicted in Figure 3.1 and let* (N, c) *denote the corresponding Upstream Responsibility game. The weights on the arcs represent the direct emissions (in some appropriate units) of the corresponding stage of the supply chain,* $a_1 = 1$*,* $a_2 = 4, a_3 = 1, a_4 = 2$ *and* $a_5 = 2$*. As the most downstream firm in the supply chain, firm* 1 *will be responsible for all the emissions in the supply chain, that is,* $c(\{1\}) = 10$*, and indeed, for any subset of firms* S*, such that* $1 \in S$*,* $c(S) = 10$*. Further,* $c(\{2\}) = c(\{2,3\}) = c(\{2,4\}) = c(\{2,3,4\}) = a_2 + a_3 + a_4 = 7$*, and* $c(\{2,5\}) = c(\{2,3,5\}) = c(\{2,4,5\}) = c(\{2,3,4,5\}) = a_2 + a_3 + a_4 + a_5 = 9$*. Firms* $3, 4,$ *and* 5 *are individually responsible only for their direct emissions as there are no upstream stages in the* *supply chain. Therefore,* $c(\{3\}) = 1$*,* $c(\{4\}) = 2$*, and* $c(\{5\}) = 2$*. Also, clearly* $c(\{3,4\}) = 3$*,* $c(\{3,5\}) = 3$*,* $c(\{4,5\}) = 4$*, and* $c(\{3,4,5\}) = 5$*. Finally,* $c(N) = 10$*, corresponds to the emissions generated by the entire supply chain. An efficient solution of the cooperative game will be an allocation vector of responsibilities,* $\{x_i\}_{i\in N}$*, such that* $\sum_{i\in N} x_i = c(N) = 10$*. In contrast, an application of the Canadian principle of upstream emission responsibility will hold a project* i *in the fossil fuel supply chain responsible for its entire upstream emissions (Canada 2016), that is,* $c(\{i\})$*. For illustrative purposes, assume that the above fossil fuel supply chain comprises of entirely new projects. Then, in the absence of an apportionment mechanism, the attributed responsibilities for projects* $\{1,2,3,4,5\}$ *shall be given by* $[10,7,1,2,2]$*, exemplifying the double-counting.*

3.2.3 Consistency

Apparently, the Davis-Maschler reduced game property (Davis and Maschler 1965), which plays a prominent role in axiomatization of solution concepts in cooperative games, is a natural property to be desired from an emission responsibility allocation scheme in fossil fuel supply chains. To explain, let us first introduce some definitions. Let (N,c) be a (cost) cooperative game, and assume, for simplicity of exposition, that the core, $\mathcal{C}(N,c)$, of (N,c) is not empty. Then, for a given non-empty coalition S and a core allocation x, the Davis-Maschler **reduced game**, $(S,\hat{c}^x_S)$ of (N,c) **on** S **at** x is given by

$$\hat{c}^x_S(T) = min\{c(T\cup Q) - x(Q) : Q \subseteq N\setminus S\}, \forall\, T\subseteq S.$$

Note that the Davis-Maschler reduced game of an Upstream Responsibility game (N,c), on S at x, can be viewed as a cooperative game modeling of a *generalized* fossil fuel supply chain wherein the firms in $N\setminus S$ have committed to assume upstream pollution responsibilities, $x_i, i\in N\setminus S$, and the remaining firms, S, are left to take advantage of these commitments as they attempt to allocate, among themselves, upstream responsibilities for the emissions of the entire supply chain.

Definition 3.1. *A solution concept* ϕ *is said to satisfy the* ***reduced game property*** *or* ***consistency*** *if for every coalition* S *and every solution point* x*, the projection,* $x^S \equiv (x_i)_{i\in S}$*, belongs to* $\phi(S,\hat{c}^x_S)$*,*

$$x\in\phi(N,c) \Rightarrow \forall\; S\subseteq N,\; x^S\equiv (x_i)_{i\in S}\in\phi(S,\hat{c}^x_S). \tag{3.3}$$

A solution concept that satisfies the reduced game property, or consistency, satisfies internal consistency which is a fundamental requirement of any allocation method, see, e.g., (Winter 2002). Indeed, consider (a single-point) solution concept, ϕ, which we would like to use as a cost allocation scheme, and suppose that we implement ϕ in two stages. In the first stage, ϕ is implemented to determine the cost allocations for members in a coalition $N \setminus S$. The environment subsequent to the first stage represents a different (reduced) game facing players in S, whose cost allocations are yet to be determined. It would be very natural, perhaps even obvious, to require that ϕ allocates the players in the reduced game exactly the same cost shares as they would have been allocated in the original game, and a solution concept satisfying this requirement is referred to as being *consistent*.

Note that, for example, in the context of emissions allocation in global fossil fuel supply chains, consistency of an allocation method is a natural requirement. Indeed, in such supply chains, different firms and projects often fall under the jurisdiction of different regulators. In these cases, it can be argued that the proposed allocation rule, implemented at a reduced supply chain which is, e.g., under the jurisdiction of the same regulator, be invariant to previous implementations of it in other jurisdictions. Consistency also contributes to simplicity of administration, one of the yardsticks identified by the Canadian government and discussed previously. Further, we note that a cross-jurisdictional review of energy regulators commissioned by the Natural Resources Canada (Stratos 2017) broadly recommends consistency and coherence across regulatory systems while designing and implementing environmental initiatives.

3.2.4 Welfare, Incentives and the Regulator's Problem

The attributed upstream responsibility, along with the manner in which it is integrated within an existing environmental policy regime by the energy regulator, has economic implications for the firms in the fossil fuel supply chain. Regulators could opt to utilize the attributed upstream responsibility to qualitatively inform the impacts of an energy project. Alternatively, they could penalize firms by requiring them to offset or they could levy a carbon penalty on the attributed emissions, either entirely, or on the part that exceeds some predetermined threshold. Carbon penalties, such as a carbon tax, are set, in principle, so as to reflect the social cost of carbon emissions and to induce firms to internalize these costs (Plambeck 2012). Similarly, offset requirements or emission thresholds are determined, in principle and in practice, by factoring in the available state-of-the art technologies, economy-wide emission targets and so forth. The regulator designs these policies to be aligned with optimal social outcomes and by doing so, arguably, ensures that compliance with these policies is the only relevant metric for the social objective. The apportionment mechanism chosen to attribute upstream emission responsibility, however, affects the incidence of the economic costs of compliance and consequently, firm-level welfare. In this paper, we consider the effects of the adopted apportionment mechanism on firm-level and supply chain welfare and on the incentives offered to firms to adopt emission-reducing technologies. The analysis is carried out in an environment where the firms are expected to pay a carbon penalty or offset the attributed emission responsibilities. That is, we assume the regulator implements a carbon penalty levied at a price p_t on the emissions attributed to each firm in the supply chain.

Firm Welfare

The baseline allocation $\bar{x}_i$ to a firm i in the fossil fuel supply chain, under the upstream responsibility principle, is given by $\bar{x}_i = c(\{i\})$. The welfare gains for a firm i upon the adoption of the emission responsibility allocation vector x, is therefore obtained by comparing it against the baseline responsibility and is given by, $\theta_i(x) = p_t\,(\bar{x}_i - x_i)$. We also observe that since we assume, as is typical in the environmental operations literature (see, for example, Caro et al. 2013) that the emissions allocated to a firm and the resulting financial penalties do not impact the revenues from their core operations, the welfare gain, $\theta_i(x)$ can be interpreted as the firm's cost savings or profit generated by the allocation mechanism x. A natural welfare requirement from a proposed emission responsibility allocation x is that it should result in non-negative welfare gains for a firm in the fossil fuel supply chain with respect to the baseline upstream responsibility policy,

$$\theta_i(x) = p_t\,(\bar{x}_i - x_i) \;\geq\; 0, \qquad \forall\, i \in N. \tag{3.4}$$

Environmental Effectiveness

We now outline here a general methodology to analyze the environmental effectiveness of a policy, such as an upstream emission responsibility mechanism, by considering the incentives it provides to adopt potentially available emission reducing technologies. Consider a technology t that has an associated abatement potential of $e(t)$ beyond the baseline business-as-usual (BAU) emissions, at a cost $c(t)$. Such technologies available to a specific firm can be represented in an abatement cost plot, or the so-called "McKinsey curve" (Enkvist et al. 2007). That is, a simple plot of available technologies to reduce emissions and their associated costs, as sketched in the left panel of Figure 3.2. In the absence of any environmental policy, it is still profitable to invest in those technologies that lie in the fourth quadrant, as they provide environmental benefits at negative cost. If the social cost of carbon is denoted by p_S and the carbon price p_t is set at p_S, then, in Figure 3.2 (left panel), any technology lying below the line $c(t) = p_S e(t)$ would be profitable. These technologies comprise the set of socially desirable investments, i.e., the cost of the technology is less than the social cost of the emission reduction from it.

Apart from levying pecuniary penalties for pollution, environmental policies, in general, aim to alter the cost structures to enlarge the set of potentially available and profitable technologies. Therefore, a natural measure of the environmental effectiveness of an allocation mechanism would be the area of the region of potentially available costly technologies that are profitable given the specific mechanism. Formally, for a firm i with baseline BAU emissions a_i, denote by $\omega_i(x)$ the area of the space of costly emission-reduction technologies that would be profitable under the allocation rule x, with a carbon price p_t. In the right panel of Figure 3.2, we sketch the technology adoption incentives offered to firm i by an allocation mechanism x, in relation to the baseline allocation, $\bar{x}$.

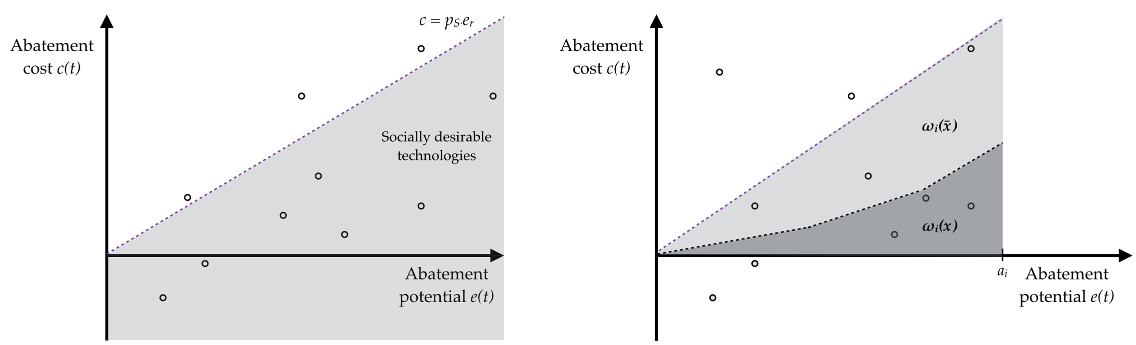


Figure 3.2: Abatement cost plot with a set of socially desirable emission reduction technologies under a carbon price $p_t = p_S$ (left panel). Technology adoption incentives for firm i by the mechanism x and the baseline allocation $\bar{x}$ (right panel).

We can extend the preceding discussion to the entire supply chain. That is, assume that each firm i in the fossil fuel supply chain has associated potentially available emission reduction technologies, denoted by $t_i = \{e_i(t_i), c_i(t_i)\}$, such that t_i can potentially achieve an emission reduction of $e_i(t_i)$ at firm i at a cost $c_i(t_i)$. For a firm i, denote the space of all potentially available emission reduction technologies, t_i, with $e_i(t_i) \in (0, a_i]$ and $c_i(t_i) \in (0, \infty)$, by $\mathcal{T}_i$. Then, the space of all emission reduction technology vectors, potentially available to the supply chain, is denoted by $\mathcal{T} = \bigoplus_{i \in N} \mathcal{T}_i$.

A vector of technologies $\mathbf{t} = \{t_i\}_{i \in N} \in \mathcal{T}$, will be adopted by the supply chain in equilibrium, under a carbon price p_t and an apportionment mechanism x, if and only if the following condition is satisfied for each $i \in N$, $\Delta_i^x(\mathbf{t}) = p_t x_i(a_i; a_{-i} - e_{-i}(t_{-i})) - p_t x_i(a_i - e_i(t_i); a_{-i} - e_{-i}(t_{-i})) \geq c_i(t_i)$, where $-i$ denotes the rest of the firms in the supply chain excluding i. Formally, denote by $\Omega(x)$ the *volume* of the n-dimensional space, $\mathcal{T}(x)$, of potentially available costly technology vectors $\mathbf{t} = \{t_i\}_{i \in N}$ that would be adopted in equilibrium under the allocation rule x and a carbon price p_t. Then,

$$\Omega(x) = \int\limits_{\substack{\mathbf{t}\in\mathcal{T} \\ \Delta_i^x(\mathbf{t})\geq c_i(t_i)}} d\boldsymbol{t} \;=\; \int\limits_{\mathbf{t}\in\mathcal{T}(x)} d\boldsymbol{t}. \tag{3.5}$$

Regulator's Problem

The regulator's problem then involves identifying an allocation mechanism x that satisfies the constraints implicitly imposed by (3.1)-(3.4) while maximizing the social objective of environmental effectiveness. The baseline allocation mechanism, $\bar{x}$, being concordant with the upstream responsibility principle, attributes each firm responsibility for its own direct emission as well as all emissions upstream to it in the supply chain. As such, it shall maximally incentivize the adoption of potentially available costly emission abatement technologies. Clearly, $\bar{x}$ is an inefficient allocation mechanism, i.e., it does not satisfy (3.1). Nevertheless, it can serve as a natural benchmark for an allocation mechanism in relation to its ability to render emission reduction technologies economically profitable. The regulator's problem can therefore be expressed as,

$$\begin{array}{ll} \max\limits_{x\in\mathbb{R}^n} & \Omega(x)/\Omega(\bar{x}) \\ \text{subject to} & (3.1)\text{ - }(3.4). \end{array}$$

In the next section, we will demonstrate that the nucleolus allocation mechanism is a feasible solution to the regulator's problem as described above. In §3.6, we will relax certain regulatory constraints and compare the environmental incentives offered by the nucleolus with respect to other feasible concordant mechanisms including the socially optimal mechanism.

3.3. The Nucleolus Allocation

Since the Upstream Responsibility game (N, c) is concave (all proofs and technical results are provided in Appendix B), we can conclude that it has a non-empty core, denoted $\mathcal{C}(N, c)$, containing the nucleolus. Therefore, the nucleolus is efficient and it induces non-negative welfares to all firms. That is, it satisfies constraints, (3.1) and (3.4) of the regulator's problem. Moreover, we note that while the Shapley value and the nucleolus both satisfy consistency, or the reduced game property, the reduced games associated with these two concepts are different. In fact, both solution concepts are axiomatized by efficiency, symmetry and the reduced game property, see, e.g., (Sobolev 1975, Hart and Mas-Collel 1989, and Winter 2002).

The Davis-Maschler reduced game, described in §3.2.3, underlies the characterization of the nucleolus. And, as elaborated previously, in the context of allocating pollution responsibilities among supply chain members, the environment representing the reduced situation for the nucleolus is very meaningful. By contrast, the reduced game underlying the characterization of the Shapley value, due to Hart and Mas-Colell (1989), is quite different, and is meaningless in the context of allocation of pollution responsibilities. In that sense, we suggest that, in fossil fuel supply chains that are subject to the upstream responsibility principle, the nucleolus is the unique "natural" single-point consistent solution mechanism to apportion supply chain emissions.

We now consider the Upstream Responsibility game (N, c), with an associated directed tree $T = (V(T), E(T))$, as introduced in the previous section. If there is a directed arc from i to j in T, we will say that the two firms, i and j, are *adjacent* in T, and that j is the successor of i in T. For such firms i and j, we denote by T_{ij} the subtree of T rooted at i away from j, consisting of all the vertices whose unique path from them to the root node contains the arc (i, j). Since each firm i has a unique successor firm j, for convenience, we sometimes also denote T_{ij} as simply T_i, and we denote the node cardinality of T_i by $|T_i|$. Further, let $a(T_{ij}) = a(T_i) \equiv a(e_i) + \sum(a(e) : e \text{ is an arc in } T_{ij})$. The following theorem leverages the coincidence of the pre-kernel and the nucleolus in concave games to characterize the nucleolus of Upstream Responsibility games. It arises from applying the pre-kernel equations, $s_{kl}(x) = s_{lk}(x)$, to pairs of adjacent players k and l in the tree.

Theorem 3.1. *A pre-imputation z in the Upstream Responsibility game (N, c) is the nucleolus if and only if z satisfies the following set of equations for each pair of adjacent players (i, j) in T, where j is the successor of i,*

$$\begin{cases} z_i = a(T_{ij}) - z(T_{ij}), \text{ if } z_j \geq a(T_{ij}) - z(T_{ij}), \\ z_i = z_j \text{ if } z_j \leq a(T_{ij}) - z(T_{ij}), \\ z(N) = c(N). \end{cases} \tag{3.7}$$

While in general, the pre-kernel equations need to be satisfied for *each* pair of distinct players, Theorem 3.1 implies that in Upstream Responsibility games, if adjacent pairs of players satisfy the pre-kernel equations, so do all the other pairs of players. Thus, it provides a characterization of the nucleolus based on *local* bargaining power considerations that only involve players that are immediate partners in the fossil fuel supply chain. That is, a pre-imputation z is the nucleolus of (N, c) if and only if $s_{kl}(z) = s_{lk}(z)$ for all adjacent players k and l in T. Theorem 3.1 also ensures that a firm which is downstream to another firm in the supply chain is necessarily assigned a larger share of the pollution responsibility by the nucleolus allocation implying that the nucleolus is concordant with the upstream responsibility principle. Further, since the nucleolus is efficient, consistent and induces non-negative firm welfares, as observed previously, we in fact have,

Theorem 3.2. *The nucleolus allocation mechanism z satisfies constraints (3.1)-(3.4) and is therefore, a feasible solution of the regulator's problem.*

We next follow Granot et al. (1996) and modify (3.7) to derive a linear-time heuristic approximation of the nucleolus, the *proto-nucleolus*, which under some conditions, as specified by Lemma 3.2 below, coincides with the nucleolus.

Definition 3.2. *The proto-nucleolus of the Upstream Responsibility game, (N, c), is a preimputation x that satisfies $x_i = a(T_{ij}) - x(T_{ij})$ for each pair of adjacent players i and j such that j is a successor of i.*

The following proposition characterizes the proto-nucleolus of Upstream Responsibility games and immediately lends itself to a linear-time computation of the proto-nucleolus.

Proposition 3.1. *The proto-nucleolus, x, of the Upstream Responsibility game (N, c) is unique and is the allocation given by*

$$x_i = \begin{cases} (a_i + \sum\limits_{k \in U_i} x_k)/2 : i \neq 1 \\ (a_1 + \sum\limits_{k \in U_1} x_k) \quad : i = 1, \end{cases} \tag{3.8}$$

where U_i denotes the set of firms immediately upstream to i.

The following proposition follows from (3.8) and the definition of the proto-nucleolus, and provides conditions for the coincidence of the proto-nucleolus and nucleolus.

Proposition 3.2. *For an Upstream Responsibility game (N, c) with proto-nucleolus x and nucleolus z,*
i. $x_i \leq x_j$ for all adjacent players i and j, where j is the successor of i, if and only if $x = z$,
ii. $a(T_{ij}) \leq a_j$ for all adjacent players i and j implies $x = z$.

Proposition 3.2 clarifies that the proto-nucleolus coincides with the nucleolus mechanism if and only if the proto-nucleolus is itself a concordant allocation mechanism. Secondly, if the direct emissions of downstream entities in the fossil fuel supply chain is sufficiently larger than their immediate upstream partners, then the proto-nucleolus will coincide with the nucleolus. We note that the proto-nucleolus is related to a pollution responsibility allocation method discussed by Gallego and Lenzen (2005). Therein, the authors propose a non-game theoretic responsibility sharing method where a fraction of the responsibility for pollution at a site is borne by the polluting firm, and a fraction is passed on to the downstream firms. Lenzen et al. (2007) illustrate the method with an example where the fraction of pollution passed to downstream firms is half. In this case, the Gallego-Lenzen allocation coincides with the proto-nucleolus, where half of the pollution, a_i, is allocated to firm i and the immediately downstream firm, in turn, is allocated a half of that and so on. Thus, the proto-nucleolus captures the intuition behind the Gallego-Lenzen method although it arises from entirely different considerations, as an approximation to the nucleolus.

The following lemma is the basis for a quadratic-time algorithm to compute the nucleolus allocation of upstream emission responsibilities in the fossil fuel supply chain. For $j \in N$, $j \neq 1$, define $c_j = \frac{a(T_j)}{|T_j|+1}$, and for $j = 1$, define $c_j = \frac{a(T)}{|T|}$.

Lemma 3.1. *Let z be the nucleolus of the Upstream Responsibility game, and let i denote a player for which c_j, $j \in N$, attains the minimum. Then, $z_l = c_i$ for all $l \in T_i$.*

Algorithm A

Step 0. Initiate with T, the weighted directed supply chain tree.
Step 1. Determine player $i \in N$ for which c_j as defined above is minimized with arbitrary breaking of ties.
Step 2. The nucleolus z allocates c_i to all players in T_i.
Step 3. Remove all nodes in T_i, that is, N is updated to $N \backslash V(T_i)$. If there are no more players, terminate the algorithm.
Step 4. Otherwise add c_i to a_j, the pollution at node j, where j is the node immediately downstream to i.
Step 5. Return to Step 1.

Lemma 3.1, coupled with the consistency property of the nucleolus, implies that Algorithm A computes the nucleolus of Upstream Responsibility games in quadratic time.

Theorem 3.3. *Algorithm A computes the nucleolus allocation mechanism z of the Upstream Responsibility game (N, c) in $O(|N|^2)$ operations.*

3.4. An Implementation Framework and Stability Analysis

The polynomial-time algorithm constructed in §3.3 is useful from a computational point of view, but necessitates central planners to use, as inputs, the direct emissions in order to compute the allocated responsibilities to each firm in the fossil fuel supply chain falling under their jurisdiction. We now complement the algorithmic approach by providing a non-cooperative policy framework that supports the implementation of the nucleolus. That is, we describe in this section simple policies with easily verifiable compliance. When these policies are imposed by the regulator on the firms in the supply chain, they ensure that profit-maximizing[3] firms, following a well-specified protocol, will uniquely organize themselves to allocate upstream supply chain emissions in accordance with the nucleolus allocation. Specifically, we consider the following two policies.

Policy $\mathcal{M}$: A firm or project in the supply chain is forbidden from bearing a smaller emission responsibility than its immediate upstream firms.

Policy $\mathcal{P}$: Each firm is permitted to collaborate with other firms in the fossil fuel supply chain to form an *alliance*, and all the firms in the alliance bear equal responsibility for, at the minimum, the upstream emissions of the alliance that have not already been accounted for by some other group. Moreover, in accordance with the notion of upstream responsibility, each alliance is permitted to transfer at most an equal upstream responsibility share to the rest of the downstream supply chain members.

Therefore, policy $\mathcal{M}$ imposes a monotonicity constraint on the implementation outcomes and naturally ensures that the emission responsibility shares that the firms are allocated in any outcome are concordant with the upstream responsibility principle. Policy $\mathcal{P}$ allows the formation of alliances in the supply chain and provides guidelines on how the firms in an alliance can share upstream emission responsibility amongst themselves.

Formally, an alliance is a subset of firms in the supply chain and an *alliance structure* is defined as $\mathcal{A} = \{A_1, ..., A_m\}$, where $\bigcup_{k=1}^{m} A_k = N$ and $A_k \cap A_l = \phi$ for $k \neq l$. We observe that each realization of Algorithm A to compute the nucleolus naturally defines a special alliance structure $\mathcal{A}^n = \{A_1^n, ..., A_m^n\}$, where each alliance in $\mathcal{A}^n$ corresponds to a specific subtree T_i obtained in some iteration of Algorithm A, and that the nucleolus allocation z complies with policies $\mathcal{M}$ and $\mathcal{P}$. Since the algorithm may encounter ties in each iteration that are broken arbitrarily, we note that the nucleolus alliance structure may not necessarily be unique for a given fossil fuel supply chain.

We next examine the space of feasible allocation vectors defined by policies $\mathcal{M}$ and $\mathcal{P}$. We begin with some illustrative examples which clarify that the policies are well-defined, verifiable in linear-time and may sometimes yield inefficient allocations.

Example 3.2. *Consider the simple supply chain depicted in Figure 3.3a with arc-weights denoting the associated direct emissions, and the alliance structure* $\mathcal{A} = \{A_1, A_2, A_3\}$ *where* $A_1 = \{1, 5\}$, $A_2 = \{2, 3\}$, $A_3 = \{4\}$. *Consider an allocation to each of the players under the alliance structure* $\mathcal{A}$ *given by the vector* $x = [2.5, 2, 2, 1, 2.5]$. *It is easily seen that the allocation vector* x *satisfies* $\mathcal{M}$ *and* $\mathcal{P}$, *which clarifies that policies* $\mathcal{M}$ *and* $\mathcal{P}$ *are well defined. However, in this example, the nucleolus alliance structure,* $\mathcal{A}^n$, *is unique and can be shown to consist of independent alliances, i.e., all alliances therein are singletons, and is therefore*

[3]Since we assume that the emissions allocated to a firm and the resulting financial penalties do not impact the revenues from their core operations, the profit of a firm given an allocation mechanism x is an affine function of its individual firm welfare, $\theta_i(x)$, and is maximized when $\theta_i(x)$ is maximized.

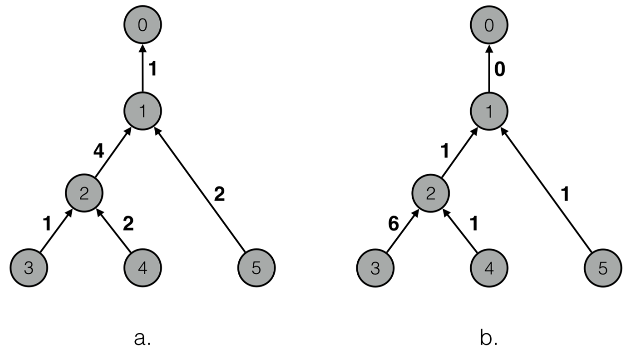


Figure 3.3: Illustrative examples with a simple supply chain and policy-compliant allocations.

distinct from $\mathcal{A}$. Further, it can be easily verified that the nucleolus allocation in this case, given by $z = [4.75, 2.75, 0.5, 1, 1]$, also complies with policies $\mathcal{M}$ and $\mathcal{P}$. Finally, note that, in general, compliance with policies $\mathcal{M}$ and $\mathcal{P}$ is verifiable in linear time.

Example 3.3. *Consider the supply chain with modified arc-weights depicted in Figure 3.3b, and the alliance structure $\mathcal{A} = \{A_1, A_2, A_3, A_4\}$, where $A_1 = \{1, 5\}$, $A_2 = \{2\}$, $A_3 = \{3\}$ and $A_4 = \{4\}$. Consider the allocation vector $x = [3, 3, 3, 0.5, 3]$. x satisfies policies $\mathcal{M}$ and $\mathcal{P}$, but it is not an efficient allocation since it over-allocates the supply chain emissions. In fact, it is easily seen that for the alliance structure $\mathcal{A}$, there does not exist an efficient allocation of the supply chain emissions that satisfies policies $\mathcal{M}$ and $\mathcal{P}$. Similarly, consider the alliance structure $\mathcal{A}' = \{A'_1, A'_2, A'_3\}$, where $A'_1 = \{1\}$, $A'_2 = \{2, 5\}$, and $A'_3 = \{3, 4\}$. Observe that $\mathcal{A}'$ contains alliances that are non-contiguous. Then, the allocation vector $x' = [7/3, 7/3, 7/3, 7/3, 7/3]$ satisfies policies $\mathcal{M}$ and $\mathcal{P}$ but it is not efficient and it is easily seen that there exists no efficient allocation vector satisfying the two policies.*

Formally, consider an alliance structure $\mathcal{A}$ and an allocation vector, x, of upstream emission responsibilities in the fossil fuel supply chain that complies with the policies $\mathcal{M}$ and $\mathcal{P}$. We now translate the two policies in terms of the constraints that they impose on x. For an alliance A, denote the set of firms in $N \backslash A$ upstream to some firm in A by $U(A)$. Policy $\mathcal{M}$ implies that for firms i and j such that i is upstream to j in the supply chain, $x_i \leq x_j$. Policy $\mathcal{P}$ then implies that for an alliance $A \in \mathcal{A}$,

$$\begin{cases} x(A) \geq c(A) - x(U(A)) - \frac{x(A)}{|A|}, 1 \notin A \\ x(A) \geq c(A) - x(U(A)), 1 \in A \\ x_i = x_j \text{ if } i, j \in A. \end{cases} \tag{3.9}$$

It is easily seen that policies $\mathcal{M}$ and $\mathcal{P}$ are well-defined, in the sense that, given any alliance structure $\mathcal{A}$, there always exist allocations that comply with the two policies. For example, given any fossil fuel supply chain and an arbitrary alliance structure, the allocation x that allocates $c(N)$ to all the members in the supply chain trivially satisfies (3.9). Moreover, for the same reason, given any alliance structure, in general, there will in fact exist infinite emission responsibility allocations that comply with policies $\mathcal{M}$ and $\mathcal{P}$. However, in Propositions 3.3 and 3.4 below, we establish that, assuming the firms in the fossil supply chain are rational, that is, profit maximizing, they will allocate responsibilities uniquely for a given alliance structure $\mathcal{A}$.

We first consider the important special case of *contiguous* alliance structures. An alliance structure, $\mathcal{A} = \{A_1, ..., A_m\}$, is said to be contiguous if the subgraphs induced by the players in each of its component alliances, $A_i \in \mathcal{A}$, are connected in the supply chain graph. For this case, we provide an explicit characterization of the unique allocation vector $x^{\mathcal{A}}$ induced by the policies $\mathcal{M}$ and $\mathcal{P}$, for a given alliance structure $\mathcal{A}$.

Proposition 3.3. *Consider a supply chain consisting of rational firms compliant with policies $\mathcal{M}$ and $\mathcal{P}$, a contiguous alliance structure $\mathcal{A}$, and players i and j such that j is the immediate downstream firm to i. Then the allocation to player j, $x_j^{\mathcal{A}}$, is given by,*

$$\begin{cases} x_j^{\mathcal{A}} = x_i^{\mathcal{A}}, \text{ if } i, j \in A_k \in \mathcal{A}, \\ x_j^{\mathcal{A}} = \max\left\{x_i^{\mathcal{A}}, \frac{a(A_k)+a(T_i)-x^{\mathcal{A}}(T_i)}{|A_k|+1}\right\} \text{ if } i \notin A_k, j \in A_k, j \neq 1 \\ x_j^{\mathcal{A}} = \max\left\{x_i^{\mathcal{A}}, \frac{a(A_k)+a(T_i)-x^{\mathcal{A}}(T_i)}{|A_k|}\right\} \text{ if } i \notin A_k, j \in A_k, j = 1. \end{cases} \tag{3.10}$$

We note that for the special case when the alliance structure arises from a situation where all firms belong to singleton alliances, the corresponding allocation $x^{\mathcal{A}}$ that complies with policies $\mathcal{M}$ and $\mathcal{P}$ coincides with the Gallego-Lenzen allocation discussed in §3.3.

We now generalize the above proposition for the case of *non-contiguous* alliance structures. That is, alliance structures that may contain alliances corresponding to disconnected subgraphs in the fossil fuel supply chain. First, we need to introduce some new definitions. A set of firms S is said to *block* another disjoint set of firms T if there exist possibly identical firms $i, j \in S$ and $u, v \in T$, such that u is downstream to i and v is upstream to j. For example, if firm i is downstream to firm u and upstream to firm v, then $S = \{i\}$ blocks the set of firms $T = \{i, j\}$.

Given an alliance structure $\mathcal{A}$ of the set of firms N, let $M_{\mathcal{A}}$ denote a set of firms which is a set-union of alliances in $\mathcal{A}$. $M_{\mathcal{A}}$ is a *minimal non-blocking set* of firms with respect to $\mathcal{A}$ if, (i) $M_{\mathcal{A}}$ is neither blocked nor does it block any alliance in $N \backslash M_{\mathcal{A}}$, and (ii) no subset of $M_{\mathcal{A}}$ satisfies (i). We define the *minimal non-blocking set structure*, $M(\mathcal{A})$, $M(\mathcal{A}) = \{M_1, ..., M_k\}$, with respect to $\mathcal{A}$, as the set of minimal non-blocking sets of firms in N, such that $\bigcup_{i=1}^{k} M_i = N$

and $M_i \cap M_j = \phi$ for $i \neq j$. It can be shown that for an alliance structure, $\mathcal{A}$, $M(\mathcal{A})$ is unique. Further, note that any set in $M(\mathcal{A})$ is either an original alliance in $\mathcal{A}$ or a union of alliances in $\mathcal{A}$, and that if $\mathcal{A}$ consists of non-blocking alliances, such as if $\mathcal{A}$ is a contiguous alliance structure, then $M(\mathcal{A}) = \mathcal{A}$. In particular, for a nucleolus alliance structure $\mathcal{A}^n$, $M(\mathcal{A}^n) = \mathcal{A}^n$.

In Proposition 3.4 below, we show that the explicit characterization provided in (3.10) for contiguous alliance structures can be generalized to non-contiguous alliance structures. In this case, the minimal non-blocking sets of alliances comprising $M(\mathcal{A})$ play the role that the individual alliances in $\mathcal{A}$ played in Proposition 3.3.

Proposition 3.4. *Consider a fossil fuel supply chain consisting of rational firms compliant with policies $\mathcal{M}$ and $\mathcal{P}$, an alliance structure $\mathcal{A}$, and players i and j in alliances $A_u, A_v \in \mathcal{A}$, respectively. Then, the unique allocation vector $x^{\mathcal{A}}$ is given by,*

$$\begin{cases} x_j^{\mathcal{A}} = x_i^{\mathcal{A}}, \text{ if } i, j \in M_k \in M(\mathcal{A}), \\ x_j^{\mathcal{A}} = \max\left\{x_i^{\mathcal{A}}, \frac{c(M_k) - x^{\mathcal{A}}(U(M_k))}{|M_k|+1}\right\} \text{ if } j \in M_k, i \in U(M_k), 1 \notin M_k \\ x_j^{\mathcal{A}} = \max\left\{x_i^{\mathcal{A}}, \frac{c(M_k) - x^{\mathcal{A}}(U(M_k))}{|M_k|}\right\} \text{ if } j \in M_k, i \in U(M_k), 1 \in M_k, \end{cases} \tag{3.11}$$

where $U(M_k)$ denotes the set of firms upstream to M_k.

From the above proposition, we immediately obtain the following corollary that if two different alliance structures have identical associated minimal non-blocking set structures, then the allocations induced by the two alliance structures are also identical.

Corollary 3.1. *For alliance structures $\mathcal{A}_1$ and $\mathcal{A}_2$ such that $M(\mathcal{A}_1) = M(\mathcal{A}_2)$, $x^{\mathcal{A}_1} = x^{\mathcal{A}_2}$.*

Although, compliance with the two policies induces an infinite set of feasible allocation vectors, Propositions 3.3 and 3.4 establish a non-injective (many-to-one) mapping between the alliance structure and its associated allocation vector for fossil fuel supply chains with rational firms. Thus, given an alliance structure $\mathcal{A}$ in a fossil fuel supply chain, we may assume that $x^{\mathcal{A}}$ is the unique allocation of responsibilities that will be induced by policies $\mathcal{M}$ and $\mathcal{P}$ imposed by the regulator. Clearly, if the alliance structure coincides with a nucleolus alliance structure, i.e., $\mathcal{A} = \mathcal{A}^n$, then $x^{\mathcal{A}} = z$, where z is the nucleolus allocation.

3.4.1 Endogenous Formation of Alliances

We are now interested in the dynamics of how firms in a fossil fuel supply chain will organize themselves subject to policies $\mathcal{M}$ and $\mathcal{P}$ being imposed by the regulator, and the alliance structures that can be expected to be formed. We therefore analyze an endogenous process of alliance formation in a fossil fuel supply chain that is mandated to assume responsibility for the total supply chain emissions. To this end, we consider a well-specified protocol, consisting of a sequential procedure of alliance formation, whereby, downstream firms are permitted to offer upstream firms to join them in their existing alliance, and in response, upstream firms can choose to either accept or reject the offer, proceeding sequentially through all the firms in the supply chain.

Formally, the protocol mandates players to choose their actions in an order ρ, proceeding sequentially upstream through the supply chain from the most downstream entity to the most upstream entities, with ties broken arbitrarily. Following the order ρ, each player j in the supply chain chooses an action o_{ji} with respect to each of its immediate upstream partners i, $o_{ji} \in \{\text{Offer, Do Not Offer}\}$. That is, to either offer or not offer i to join the alliance that j is currently a member of, denoted by {O,D} in Figure 3.4. If player j chooses to offer player i to join the alliance, then i can choose an action $a_{ij} \in \{\text{Accept, Reject}\}$. That is, to either accept or reject j's offer, denoted by $\{A, R\}$, respectively, in Figure 3.4. If j chooses to not offer membership to i, then we vacuously allow i to reject j's non-existent offer.

For a given fossil fuel supply chain represented by the directed tree T, vector of arc-weights a, and the order ρ, we can therefore define a sequential game with perfect information, the *alliance formation game*, $\Gamma(T, a, \rho)$, which can be represented by a game tree $H(\Gamma)$, as, for example, depicted in Figure 3.4. For each node t in the game tree H, the subtree rooted at t corresponds to a subgame Γ_t of the alliance formation game, Γ. The history of the game at node t, denoted by $H_t(\Gamma)$, consists of the players who have already played prior to t, $N(H_t)$, their corresponding sequence of actions, $A(H_t)$, and the player, $n(H_t)$, who is to choose the immediate next action.

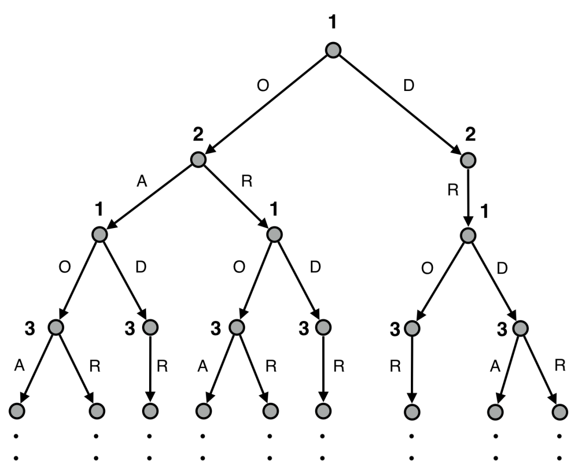


Figure 3.4: Game tree $H(\Gamma)$ corresponding to an alliance formation game Γ in a typical fossil fuel supply chain.

A strategy profile, $\sigma = \{\sigma_i\}_{i \in N}$, is a mapping, for each player i, from all subgames Γ_t such that $i = n(H_t)$, to a feasible action for i. Each strategy profile σ results in a unique path of actions, $\pi(\sigma)$, from the root node to a leaf node of the game tree H, which is the outcome of the alliance formation game Γ played with strategy profile σ, and $\pi(\sigma)$ generates the alliance structure, $\mathcal{A}(\sigma)$. The precise payoffs, that is, the allocation of responsibilities within the alliance structure, $\mathcal{A}(\sigma)$, is governed by the policies $\mathcal{M}$ and $\mathcal{P}$, which can be thought of as exogenous constraints on the allocations. As observed earlier, assuming the firms in the fossil fuel supply chain are profit-maximizing, the resulting unique allocation of responsibilities is given by $x^{\mathcal{A}(\sigma)}$, characterized in Proposition 3.3. Note that it is indeed possible, as in Example 3.3, that the allocation may not always be efficient, in the sense that, the formation of certain alliance structures may necessarily result in an allocation that over-allocates the supply chain emissions.

The central question of interest is, of the many possible alliance structures, which ones would be formed by the firms. We expect the alliance structures that will form to be those which are generated by equilibrium strategy profiles in the alliance formation game. In that respect, the following result provides a basis for the endogenous formation of those alliance structures that yield the nucleolus allocation, thereby providing an implementation framework. In other words, the result below provides a non-cooperative implementation of the nucleolus mechanism to apportion upstream emission responsibility.

Theorem 3.4. *The alliance structure generated by any subgame perfect equilibrium strategy profile $\tilde{\sigma}$ of the alliance formation game $\Gamma(T, a, \rho)$ is a nucleolus alliance structure, $\mathcal{A}(\tilde{\sigma}) = \mathcal{A}^n$.*

3.4.2 Stability of Alliance Structures

We now adopt a complementary perspective that allows us to analyze the stability of alliance structures under the policies $\mathcal{M}$ and $\mathcal{P}$. In order to do so, we employ an approach based on the strong Nash equilibrium concept, according to which an individual player, or a group of players, can withdraw from their current alliance and form a new alliance if the deviation makes all players in the group strictly better off. We proceed to delineate the mechanics of a deviation. Formally, given an alliance structure $\mathcal{A}$, and the corresponding allocation vector $x^{\mathcal{A}}$, consider a set of firms $S \subset N$ in the supply chain. A deviation by S from the alliance structure $\mathcal{A}$ results in a new alliance structure containing the alliance comprising the firms in S along with the previous alliances in $\mathcal{A}$ excluding those members now in S. We note that, in general, the original alliance structure as well as the alliance structure arising from a deviation by S, may be non-contiguous. Therefore, this approach allows us to extend the implicitly imposed sequential communication structure in Theorem 3.4 which permitted only partner firms to form alliances.

An alliance structure $\mathcal{A}$ is said to be *strong Nash-stable* if no set of firms S in the supply chain has a strictly profitable deviation. That is, there is no alliance structure $\mathcal{B}$ resulting from a deviation of S from $\mathcal{A}$, for which $x_i^{\mathcal{B}} < x_i^{\mathcal{A}}$ for all $i \in S$. In the case of the simple supply chain considered in Example 3.2, though the alliance structure $\mathcal{A}$ complies with policies $\mathcal{M}$ and $\mathcal{P}$, it is not strong Nash-stable because player 5, for example, can feasibly and profitably deviate from the alliance $\{1, 5\}$ to form the singleton alliance $\{5\}$, and reduce its allocation from 2.5 to 1. We are interested in identifying the allocations induced by alliance structures that are strong Nash-stable in a fossil fuel supply chain subject to the policies $\mathcal{M}$ and $\mathcal{P}$.

The following result allows us to restrict our attention to contiguous alliance structures since for each non-contiguous alliance structure that is strong Nash-stable, there exists a strong Nash-stable contiguous alliance structure that yields an identical allocation of responsibilities.

Lemma 3.2. *Consider a non-contiguous strong Nash-stable alliance structure $\mathcal{A}$. Then, there exists a contiguous strong Nash-stable alliance structure, $\mathcal{A}'$, such that $x^{\mathcal{A}} = x^{\mathcal{A}'}$.*

The following theorem, in turn, shows that all contiguous strong Nash-stable alliance structures correspond to a nucleolus alliance structure and therefore result in an identical allocation of responsibilities that coincides with the nucleolus allocation.

Theorem 3.5. *A contiguous alliance structure $\mathcal{A}$ is strong Nash-stable under policies $\mathcal{M}$ and $\mathcal{P}$ if and only if $\mathcal{A} = \mathcal{A}^n$. Then, $x^{\mathcal{A}} = z$, where z is the nucleolus allocation.*

The above theorem demonstrates that the only contiguous strong Nash-stable alliance structures are nucleolus alliance structures. However, by Lemma 3.2 we immediately obtain that all other alliance structures that are strong Nash-stable also result in identical allocation of emission responsibilities as in a nucleolus alliance structure.

The stability analysis performed here complements the implementation framework developed in §3.4.1. It speaks to the ability of the relatively straightforward and easily verifiable policies, $\mathcal{M}$ and $\mathcal{P}$, to sustain the nucleolus mechanism to allocate upstream emissions in a fossil fuel supply chain.

3.5. Structural Properties and Implications

In this section, we establish certain structural properties of the nucleolus alliance structure, and equivalently, of the nucleolus allocation mechanism to apportion upstream emission responsibility in fossil fuel supply chains. These properties assume significant importance in policy-contextual modelling, such as ours, as it reaffirms the operational validity of the proposed approach (Gass 1983). Motivated by our theoretical results, we further highlight their practical implications in terms of rationalizing the interpretability and applicability of the nucleolus mechanism.

In §3.4, we prescribed policies that provide an implementation framework for the nucleolus allocation mechanism. In certain situations, the most downstream player in a fossil fuel supply chain corresponds to the consumers, and it may prove infeasible to include the consumers in an implementation mechanism such as the one described. However, Proposition 3.5 reveals that the most downstream entity always forms a singleton alliance, as long as its activities generate a non-zero pollution. Therefore, in almost all realistic situations, this player can be removed from the implementation procedure without any consequence.

Proposition 3.5. *For any fossil fuel supply chain with $a_1 > 0$, a nucleolus alliance structure, $\mathcal{A}^n$, contains the singleton alliance, $\{1\}$.*

We now proceed to investigate the effects of changes in emissions at some stage of the fossil fuel supply chain on the nucleolus allocation z. An allocation mechanism that is too sensitive to small changes in the emission outputs in various stages of the supply chain is undesirable practically. Transparent mechanisms that lend themselves to simple sensitivity analyses are easier to implement from a regulatory perspective, and are likely to be viewed by the participating firms as being fairer. In general cooperative games, it is well-known that the nucleolus is piecewise linear in the characteristic cost function (e.g., Charnes and Kortanek 1969). However, such a result is not directly applicable to our setting because we are interested in the effect of changes in the emissions at some stage in the supply chain, which is an underlying "primitive" of the derived cooperative game. Consider firms i and j in a fossil fuel supply chain (i and j may be identical), and let z be the nucleolus allocation of the associated upstream emission responsibility cooperative game.

Proposition 3.6. *The nucleolus allocation to firm i, z_i, is continuous piecewise linear and non-decreasing in the direct emissions of firm j, a_j.*

Proposition 3.6 reveals that the effects of small changes in emissions at different stages on the responsibilities allocated to the firms are linear, thereby emphasizing the transparency of the nucleolus allocation mechanism. We now study the effect of larger increases in emissions of a particular project in the fossil fuel supply chain. Consider a project j whose emissions increases from a_j to $a_j + \Delta$. For sufficiently large Δ, we are able to provide an explicit characterization of the nucleolus alliance structures.

Specifically, let P_j denote the set of firms in the supply chain on the unique path from firm j to the root node 1, including j but excluding 1. Let L denote the set of firms that are not in P_j but adjacent to a firm in P_j, again excluding the root node 1. It is easily seen then that $N = P_j \bigcup \{1\} \bigcup_{k \in L} V(T_k)$, where recall that T_k denotes the subtree of T rooted at

k. Given a subtree T_k, $k \in L$, let $\mathcal{A}_k^n$ denote a nucleolus alliance structure of the sub-supply chain restricted to the subtree spanned by $V(T_k) \cup k'$, where k' is the root node of sub-supply chain with $k' \in P_j$ and adjacent to k.

Proposition 3.7. *Consider a firm j in a fossil fuel supply chain with associated direct emissions $a_j + \Delta$. Then, for sufficiently large Δ, any nucleolus alliance structure, $\mathcal{A}^n$, is given by $\mathcal{A}^n = \{\{1\}, P_j, \{\mathcal{A}_k^n\}_{k \in L}\}$, and further, $\frac{\partial z_i}{\partial \Delta} = 0$ where z_i is the nucleolus allocation to $i \in T_k,\ k \in L$.*

Proposition 3.7 provides an explicit characterization of a nucleolus alliance structure when the increase in emissions, Δ, is sufficiently large. Moreover, it reveals that beyond some threshold, the nucleolus allocation mechanism attributes responsibility for a large marginal increase in the direct emissions associated with a particular project in the supply chain, such as, for example, substantial capacity expansion, only to the firms directly downstream to that particular project.

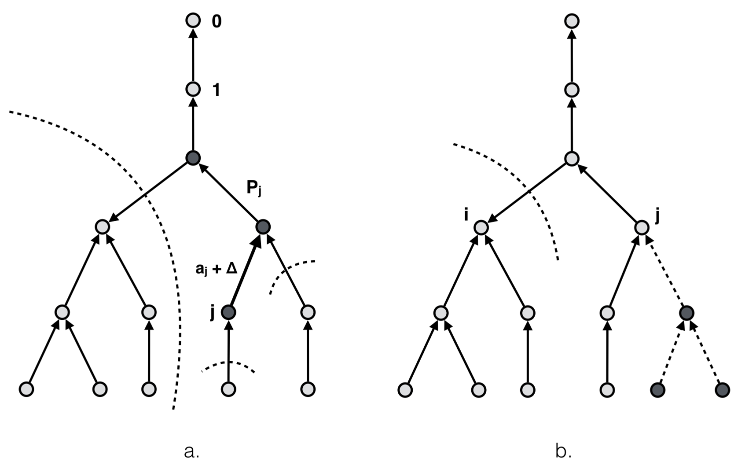


Figure 3.5: Illustrating the structural properties of the nucleolus allocation mechanism (Example 3.4).

Finally, we consider the effects of very general arbitrary structural changes in the supply chain network, for example, the addition of new projects such as extractors or refineries, disaggregation or closure of existing supply chain members and so forth. Formally, consider a fossil fuel supply chain enterprise, $\mathcal{SC} = (V, E, a, N)$, and recall from §3.2.2 that V and E are the vertex and edge sets of the directed tree representation, T, of the supply chain enterprise $\mathcal{SC}$. N denotes the set of firms in the supply chain, and $a : E \to \mathbb{R}$ is an edge-weighting that associates the direct emissions corresponding to each stage of the fossil fuel supply chain. A supply chain enterprise $\mathcal{SC}' = (V', E', a', N')$ represented by a directed tree T', is said to be obtained by a *structural change* to $\mathcal{SC}$ at $S \subset N$, if $N \backslash S \subseteq N'$, and the weighted sub-trees induced by the firms in $N \backslash S$ in T and T', respectively, are identical. As defined, a structural change therefore encompasses changes to the underlying graphical structure of the supply chain via either addition of new firms, removal of existing firms, or changes in the supply chain linkages, as well as changes to the direct emissions associated with particular stages of the supply chain. Now, let us consider an alliance, A_k^n, belonging to a nucleolus alliance structure, $\mathcal{A}^n$, of the supply chain enterprise $\mathcal{SC}$.

Proposition 3.8. *The nucleolus allocation to firms in the alliance $A_k^n \in \mathcal{A}^n$ does not increase due to structural changes in the supply chain that are not upstream to any member of that alliance.*

Proposition 3.8 notes that the nucleolus allocation to a firm can increase only as a consequence of structural changes that are upstream to some firms in the alliance that it belongs to. Changes to the supply chain network that are either downstream, or in other sub-supply chains that are not upstream to any firm in the alliance a firm belongs to, can only decrease or leave unaffected the emission responsibility allocated to that firm. Apart from ensuring ease of interpreting the effects of structural changes, Proposition 3.8 re-emphasizes the adherence of the nucleolus allocation mechanism to the underlying principle of upstream responsibility which mandates fossil fuel firms to bear responsibility only for upstream emissions.

Example 3.4. *Consider the supply chain depicted in the left panel of Figure 3.5. Proposition 3.5 implies that a nucleolus alliance structure, $\mathcal{A}^n$, contains the singleton alliance consisting of the most downstream entity in the supply chain, $\{1\}$. Proposition 3.7 demonstrates that when the increase Δ in the direct emissions of firm j, $a_j + \Delta$, is sufficiently large, then j and firms that are intermediate to j and the downstream entity 1 all belong to the same alliance, P_j in $\mathcal{A}^n$. Finally, consider the supply chain represented in the right panel of Figure 3.5. For $i \in A_k^n \in \mathcal{A}^n$, a structural change to the supply chain at $S \subset N$ that is upstream to firm j, such that j is not downstream to any firm in A_k^n, will not increase the allocation to firms in $V(T_i)$ according to Proposition 3.8.*

3.6. Fairness, Welfare and Incentive Considerations

In this section, we consider a regulator implementing a carbon penalty levied at a price p_t on the emissions attributed to each firm in the supply chain as described in §3.2.4. The welfare gains for a firm i upon the adoption of the emission responsibility allocation vector x, is then given by, $\theta_i(x) = p_t\,(\bar{x}_i - x_i)$. Thus, the welfare of the overall supply chain given the allocation x, is $\Theta(x) = \sum\limits_{i \in N} \theta_i(x)$, and therefore, for all efficient allocation mechanisms x, $\Theta(x) = p_t(\sum\limits_{i \in N} c(\{i\}) - c(N)) \equiv W$, a constant. Thus, under an emission penalties policy regime, every efficient emission responsibility mechanism including the nucleolus, not surprisingly, attains identical supply chain welfare[4].

However, different responsibility apportionment mechanisms distribute the net welfare differently across the supply chain. A report commissioned by the Natural Resources Canada to review energy regulators within Canada and internationally (Stratos 2017) observes that a fair distribution of costs across the economy engenders trust and fosters participatory decision making. Further, as noted previously, fairness is one of the five yardsticks recommended by the Canadian government to evaluate environmental policy proposals. This, therefore, calls for a formal conceptualization that can evaluate the fairness of the distribution of the regulatory burden.

Lexicographic Fairness We consider a criterion, briefly introduced in §3.2, based on the Rawlsian notion of distributive fairness. For a set of firms S in the fossil fuel supply chain, consider the vector of welfares across subsets of firms in S induced by the allocation of responsibilities x, $\Theta(S,x) = (\theta(T,x))_{T \in 2^S}$, in which the welfares are arranged in an increasing order. Lexicographic fairness is achieved by maximizing the welfare of the least well-off set of firms, and then subsequently, maximizing the welfare of the second least well-off set, and so forth. This embodies the Rawlsian approach to fairness and has been previously employed in the operations literature (see, for example, Singh and Scheller-Wolf 2018). More recently, lexicographic fairness rules have also been adopted in the machine learning and mechanism design literature (e.g., McElfresh and Dickerson 2017).

Proposition 3.9. *The nucleolus allocation is the unique efficient emission responsibility allocation mechanism that induces non-negative welfares and distributes the regulatory costs borne by the firms in N in a lexicographically fair manner.*

Welfare Gains and Abatement Incentives

Beyond the implications of the apportionment mechanism on the fairness of the distribution of the economic burden on the supply chain, it can also be analyzed via its effects on the welfare gains delivered to each individual firm. To that end, in Theorem 3.6, we provide lower bounds on the welfare gains, $\theta_i(z) = p_t\,(\bar{x}_i - z_i)$, provided by the nucleolus allocation mechanism, z, in relation to the baseline allocation mechanism $\bar{x}$, $\bar{x}_i = c(\{i\})$ that, as noted previously, attributes all upstream emission responsibility to each firm in the supply chain.

[4] In this paper, we consider a regulator that collects a carbon penalty from each firm based on the attributed emissions. If instead, the upstream emissions attributed to a firm are compared against a threshold for rejection, or if the firms are expected to offset only the portion of emissions that exceeds the threshold, then the supply chain welfare will not be invariant across all efficient allocation mechanisms. The supply chain welfare will then depend on the allocation mechanism used as well as the thresholds determined by the regulator.

Since we further assume, as is typical in the environmental operations literature (see, for example, Caro et al. 2013) that the emissions allocated to a firm and the resulting financial penalties do not impact the revenues from their core operations, the bounds can therefore also be interpreted as bounds on the costs savings delivered to firms due to our allocation mechanism z.

Moreover, in Theorem 3.6, we also provide guarantees in terms of lower and upper bounds on the ability of the nucleolus allocation to render potentially available emission reduction technologies profitable for a specific firm beyond the business-as-usual emissions. That is, we bound the technology adoption incentive ratio for firm i, $\omega_i(x)/\omega_i(\bar{x})$ between an allocation mechanism x, and the baseline allocation, $\bar{x}$, as introduced in §3.2.4.

Consider a fossil fuel supply chain with the set of firms N, and a corresponding emissions profile $(a_i; a_{-i})$. Let $A(i)$ denote the alliance containing i that belongs to the nucleolus alliance structure derived by Algorithm A. Now, we recall that for an alliance A, $U(A)$ denotes the set of firms in N that are either in A or are upstream to some firm in A, and U_i denotes the set of firms immediately upstream to firm i. Finally, let $\mathbb{I}_{i\neq 1}$ represent the indicator function denoting whether $i \neq 1$.

Theorem 3.6. *Consider a firm $i \in N$ in the fossil fuel supply chain, and let z denote the nucleolus allocation. Then,*

$$\begin{cases} \theta_i(z) \geq p_t\bar{x}_i\Big(1 - \dfrac{1}{|A(i)\cap T_i| + \mathbb{I}_{i\neq 1}}\Big) \\ \theta_1(z) \geq p_t\Big(\dfrac{\bar{x}_1 - a_1}{2}\Big) \\ \theta_i(z) \geq p_t\mathbb{I}_{i\neq 1}\Big(\dfrac{3\bar{x}_i - a_i}{4} - \dfrac{\max_{j\in U_i} a_j}{12}\Big), \end{cases} \quad \textit{and} \quad \frac{1}{|U(A(i))|+1} \leq \frac{\omega_i(z)}{\omega_i(\bar{x})} \begin{cases} \leq \frac{1}{2} \ \textit{if } i \neq 1, \\ = 1 \ \textit{if } i = 1. \end{cases}$$

Theorem 3.6 provides lower bounds on the welfare gains, or equivalently cost savings, delivered to firm i by adopting the nucleolus mechanism to apportion upstream emission responsibility in relation to the baseline attribution mechanism. In particular, it provides two distinct approaches to compute the lower bounds, one in terms of the nucleolus alliance structure, and the other that is independent of it. Qualitatively, we immediately obtain, for example, that in supply chains where the most upstream emissions are relatively larger than the other direct emissions, the lower bound on the welfare delivered to firm 1 by the nucleolus mechanism, compared to the penalty imposed on it by the baseline mechanism, $p_t\bar{x}_1$, is approximately 1/2. Similarly, from the third inequality, for any firm $i \neq 1$ that is sufficiently downstream, the lower bound on the welfare delivered by the nucleolus, compared to the baseline penalty, is approximately 3/4. Further, in these supply chains, since the nucleolus alliance containing i, $A(i)$, will include all firms in the subtree rooted at i, T_i, the first inequality implies that the lower bound on the welfare delivered by the nucleolus can be strengthened to $|T_i|/(|T_i| + 1)$ of $p_t\bar{x}_i$. Moreover, Theorem 3.6 also provides guarantees in terms of lower and upper bounds on the ability of the nucleolus allocation to render potentially available emission reduction technologies profitable for a specific firm in the supply chain. For $i = 1$, the nucleolus mechanism captures the incentives offered by the baseline mechanism fully, while for firms $i \neq 1$, it incentivizes the adoption of at most half the space of potentially available technologies as compared to the baseline mechanism. We note that these upper bounds obtained in Theorem 3.6 are for general situations where we have no a priori information on the available set of technologies and hence they are assumed to lie anywhere arbitrarily on the abatement cost plot.

Recall that $\Omega(x)$ denotes the *volume* of the space, $\mathcal{T}(x)$, of potentially available costly technology vectors $\mathbf{t} = \{t_i\}_{i \in N}$ that would be adopted in equilibrium under the allocation rule x. Since, all efficient allocation rules yield identical supply chain welfare in an emissions penalty regime, then, if p_t is set at the social cost of carbon p_S, the socially optimal allocation rule concordant with the upstream emission responsibility principle maximizes $\Omega(x)$. That is, $x^* = \arg\max_{x \in \mathcal{C}} \Omega(x)$, where $\mathcal{C}$ denotes the space of efficient and concordant allocation rules, and we note that herein we relax the consistency constraint in the regulator's optimization problem as formulated in §3.2.4. Unfortunately, the socially optimal allocation mechanism, x^*, is difficult to characterize. Computing the socially optimal allocation for a given emissions profile, $\{a_i : i \in N\}$, in fact, involves jointly identifying x^* for all emission profiles, $\{b_i : b_i \leq a_i, i \in N\}$. This renders the computation of x^* intractable even for small instances and consequently, impractical to implement in practice.

Similarly, the non-separability of the nucleolus allocation to firms in the profile of emissions across the supply chain, renders the characterization of the space of profitable technologies for the entire supply chain under the nucleolus allocation challenging. We are nevertheless able to leverage a decomposition property to once again provide reasonable bounds on the performance of the nucleolus mechanism in relation to the incentives provided by the baseline allocation mechanism.

Consider the supply chain tree T with k (≥ 1) firms that are immediately upstream to firm 1, which we recall, is the most downstream firm in the supply chain. Then, the nodes corresponding to the firms in the supply chain can be partitioned as $V(T) = \{1\} \bigcup_{i \in U_1} V(T_i)$.

Theorem 3.7. *Consider a fossil fuel supply chain represented by the directed tree T and let z denote the nucleolus allocation mechanism. Then,*

$$\frac{\Omega(z)}{\Omega(\bar{x})} \geq \frac{1}{1 + \max_{i \in U_1} |T_i|}.$$

We note that for given specific supply chain configurations, the bounds derived above can be tightened by exploiting their structural features. Now, in order to further clarify the environmental outcomes offered by the nucleolus allocation mechanism z from the regulator's perspective, we analyze its relative performance as compared to two other salient allocation mechanisms for certain limit supply chain configurations. First, we consider the socially optimal efficient and concordant mechanism x^* described previously. Second, we consider an emission allocation mechanism studied in Gopalakrishnan et al. (2018), the Shapley mechanism, denoted by x^S, which attributes an equal share of the direct emissions a_i of an entity i to all firms downstream to i. We note that x^* and x^S will, in general, not satisfy the notion of consistency and are therefore feasible solutions of the regulator's optimization problem only upon relaxing this constraint.

Consider a fossil fuel supply chain, $\mathcal{SC} = (V, E, a, N)$, where $V = N \cup \{0\}$ and E are the vertex and edge sets, respectively, of the directed tree T representing the supply chain. Let S_k denote the *star tree* structure for a supply chain with $k+1$ firms with directed arcs leading from k upstream nodes to a single downstream node 1. Further, consider a potentially available technology vector $\mathbf{t} = \{t_i\}_{i \in N} \in \mathcal{T}(x)$, where recall that $\mathcal{T}(x)$ corresponds to the n-dimensional space of potentially available costly technology vectors that would be adopted in equilibrium under the allocation rule x and a carbon price p_t. To clarify, $\Omega(x)$ denotes the volume of $\mathcal{T}(x)$. Then, let $a(\mathbf{t}) = \sum\limits_{i \in N} (a_i - e_i(t_i))$ correspond to the entire supply chain's emissions upon adoption of the technology vector $\mathbf{t}$.

Theorem 3.8. *Consider a fossil fuel supply chain represented by the weighted directed tree T. Let x^*, x^S, and z, denote the socially optimal concordant mechanism, Shapley mechanism and the nucleolus mechanism respectively.*
(i) Suppose $T = S_k$, then $\Omega(x^S) = \Omega(z) \leq \Omega(x^*)$,
(ii) Suppose $a(T_{ij}) \leq a_j$ for all adjacent players $i, j \in N$, then $\Omega(x^S) \leq \Omega(z) < \Omega(x^*)$,
(iii) Suppose that for some $i \in N$, $a_i \to \infty$, then for each $\mathbf{t}^* \in \mathcal{T}(x^*)$, there exist $\mathbf{t}^{\mathbf{S}} \in \mathcal{T}(x^S)$ and $\mathbf{t}^{\mathbf{z}} \in \mathcal{T}(z)$ such that $\lim\limits_{a_i \to \infty} a(\mathbf{t}^{\mathbf{S}})/a(\mathbf{t}^*) = \lim\limits_{a_i \to \infty} a(\mathbf{t}^{\mathbf{z}})/a(\mathbf{t}^*) = 1$.

Theorem 3.8 demonstrates that for supply chains in a star configuration, the volume of the space of technology vectors incentivized for adoption by the nucleolus and Shapley mechanisms coincide. For supply chains where the direct emissions are sufficiently increasing downstream, the nucleolus outperforms the Shapley mechanism. Naturally, in both cases, these two allocations are outperformed by the socially optimal concordant mechanism. Finally, in supply chains, where the direct emissions of some entity is sufficiently large, then for each technology vector supported in equilibrium by the socially optimal mechanism, there exists equivalent technology vectors that will be supported in equilibrium by the nucleolus and Shapley mechanism achieving identical net supply chain emissions.

3.7. Case Study – Trans Mountain Pipeline System

The Trans Mountain Pipeline (TMPL) is an oil pipeline network in Western Canada from Edmonton to Burnaby that provides Alberta's oil sands access to Pacific shipping routes via the ports of the province of British Columbia. A recent controversial proposal to nearly triple its nominal capacity from the current capacity of 300,000 barrels/day to 890,000 barrels/day has run into significant opposition primarily on the basis of its environmental impacts. Canada's extensive oil sands account for 14% of global oil reserves (O&GJ 2004) and an expansion of the TMPL opens up economically lucrative shipping routes for the crude oil extracted from Alberta's oil sands. However, oil sands have often been the target of environmental groups since the life-cycle carbon emissions associated with oil sands is higher than from conventional crude oil, largely arising from higher emissions in the extraction, transportation and refining stages. In the following emissions accounting study, we focus on seven in-situ[5] oil sands and heavy oil projects that are expected to contribute around 224,500 bbl/day of capacity between 2016 and 2019 (ECCC 2016). Transported via the TMPL, the bitumen is then to be shipped via the Westridge Marine Terminal in Burnaby, British Columbia, and exported to refineries in the Asia-Pacific region.

As previously discussed, the Canadian federal government, since 2016, has a stated objective of factoring in upstream emissions associated with a project during its environmental impact assessment and in setting emission reduction targets for individual energy projects. In this section, based on available data and estimates, we provide a well-to-wheel (WTW) accounting of the emissions associated with the different stages of the fossil fuel supply chain corresponding to the TMPL expansion project. We then illustrate a practical application of our proposed nucleolus mechanism to attribute upstream emission responsibilities to individual entities in the supply chain and discuss its implications in this particular context.

The map[6] and a schematic of the fossil fuel supply chain associated with the TMPL are depicted in Figure 3.6. The direct emissions associated with each stage in the above supply chain, represented as arc weights in our game-theoretic model, are provided in Table 3.1. The assumptions and approximations that went into the carbon footprint computations are described in Appendix C and are largely based on data and estimates provided in ECCC (2016) and Charpentier et al. (2009). From our carbon footprinting analysis (Table 3.1), we find that the supply chain associated with the oil sands and the TMPL has a carbon footprint of 105.54 kiloton (kt) CO_2Eq/day, and we observe that the extraction emissions accounts for around 17% of the total supply chain emissions, which is in line with estimations from

[5] In-situ mining is one of two main methods of recovering the deposits, the other being surface mining for shallower mines. Dyer and Huot (2010) estimate that 80% of Alberta's oil sands necessitate in-situ mining and is associated with two and half times as much emissions per barrel of bitumen as surface mining.

[6] Trans Mountain Jet Fuel and Trans Mountain Puget Sound are two further re-routings of the TMPL which we omit from our case study.

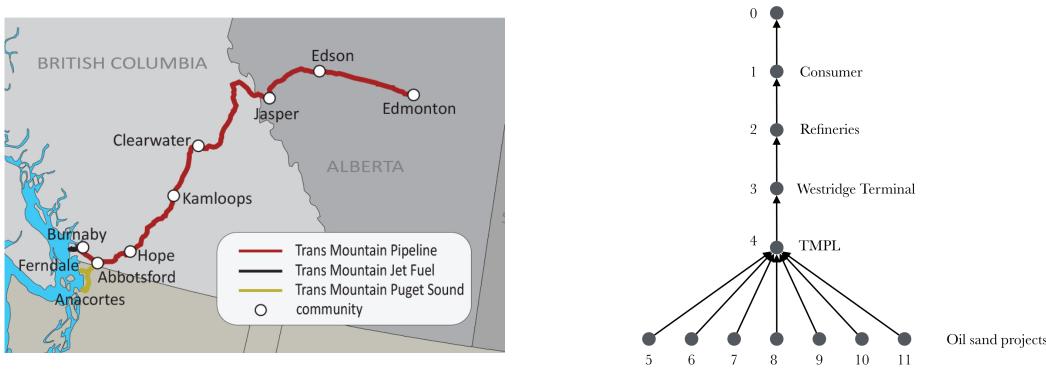


Figure 3.6: A map of the Trans Mountain pipeline expansion project and a schematic of the supply chain associated with the pipeline.

other similar sources (Charpentier et al. 2009). Further, the largest share of greenhouse gas emissions in the supply chain, around 66%, expectedly arises from the eventual downstream combustion of the extracted fossil fuel. The direct emissions associated with the intermediate projects, the TMPL expansion and the Westridge Terminal, account only for a minor portion of the total supply chain emissions.

The responsibility allocations to the entities in the fossil fuel supply chain in accordance with the nucleolus mechanism can now be computed using the algorithm presented in §3.3, both in absolute terms and as a percentage of the total emissions associated with the supply chain, and are also provided in Table 3.1. Responsibility allocations corresponding to three alternative mechanisms that are also concordant with the upstream responsibility principle are considered. The first is the baseline, or the total upstream responsibility (TUR) mechanism, $\bar{x}$, discussed in §3.2, that double counts and holds each entity responsible for all associated upstream emissions. Secondly, since the total upstream responsibility mechanism is inefficient, we consider a natural adjustment to the TUR mechanism, the adjusted total upstream responsibility (Adjusted TUR) mechanism, $\bar{x}^{\mu}$, that identifies a scaling factor μ rendering the mechanism efficient. That is, $\bar{x}_i^{\mu} = x/\mu$, where,

$$\mu = \frac{\sum_{i \in N} \bar{x}_i}{c(N)}. \tag{3.12}$$

Third, we compute the Shapley mechanism discussed in §3.6. Comparing the four different allocations, we qualitatively observe some salient features. The TUR mechanism, as well as the Adjusted TUR mechanism, attribute a relatively much larger responsibility to the TMPL, the main entity of interest in the supply chain. This explains the environmental NGOs' preference for the TUR method. However, the nucleolus allocation, which incorporates the principle of upstream responsibility across the supply chain and was shown to be consistent in a well-defined sense and to fairly distribute the regulatory burden across the supply chain, only allocates TMPL responsibility for 2.79% of the total supply chain emissions.

Supply Chain Member	Direct Emissions	TUR (Baseline)		Adjusted TUR		Nucleolus Mechanism		Shapley Mechanism	
Consumers	69.914	105.537	54.86%	57.898	54.86%	80.562	76.34%	82.580	78.25%
Refineries	18.350	35.623	18.52%	19.543	18.52%	10.648	10.09%	12.666	12.00%
Westridge Terminal	0.186	17.273	8.98%	9.476	8.98%	2.947	2.79%	3.491	3.31%
TMPL	0.227	17.087	8.88%	9.374	8.88%	2.947	2.79%	3.429	3.25%
West Ells	0.533	0.533	0.28%	0.292	0.28%	0.266	0.25%	0.107	0.10%
Vawn	0.751	0.751	0.39%	0.412	0.39%	0.375	0.36%	0.150	0.14%
Edam East & West	1.089	1.089	0.57%	0.598	0.57%	0.545	0.52%	0.218	0.21%
Hangingstone Expansion	2.148	2.148	1.12%	1.179	1.12%	1.074	1.02%	0.430	0.41%
Christina Lake Phase F	5.362	5.362	2.79%	2.942	2.79%	2.681	2.54%	1.072	1.01%
Foster Creek Phase G	3.222	3.222	1.67%	1.768	1.67%	1.611	1.53%	0.644	0.61%
Mackay River Phase I	3.755	3.755	1.95%	2.060	1.95%	1.877	1.78%	0.751	0.71%

Table 3.1: GHG emissions estimation for each stage in the fossil fuel supply chain and the comparison of four alternative concordant allocation mechanisms (unit: kt CO_2Eq/day). The emissions estimation only accounts for seven in-situ oil sands and heavy oil projects that are expected to contribute around 224,500 bbl/day of capacity between 2016 and 2019.

Further, all mechanisms based on the upstream emission responsibility principle shift a significant portion of the responsibility for upstream emissions downstream, leaving the upstream oil sands projects to bear a lower responsibility relative to other entities. In fact, the oil sands are nearly allocated identical relative responsibilities by three of the mechanisms. Environmental activists and regulators must take note that pushing for extended upstream emission responsibility across the supply chain might result in certain key entities in the supply chain, such as the upstream oil sands projects, being accorded a smaller relative responsibility. This is particularly acute when the Shapley mechanism is employed to correct double counting. The nucleolus allocates to the TMPL, the Westridge Terminal and the end consumers a larger responsibility than their own direct emissions, while the refineries and the oil sands are allocated smaller responsibilities. Further, the nucleolus, in fact, allocates equal responsibility to both the TMPL and the Westridge Terminal entities, thereby providing some basis for recent efforts by NGOs and activists to also focus on bringing intermediate supply chain entities such as shipping terminals used to transport fossil fuels into the discussion on climate change (Harrison 2015). We note that since mechanisms concordant with the upstream responsibility principle shift the economic burden downstream towards end-consumers and other entities possibly situated in different jurisdictions, the distributional ramifications of these mechanisms warrant more in-depth attention in future work.

Numerical Analysis

We now proceed, as part of the case study, to numerically analyze the environmental and economic consequences of adopting the nucleolus mechanism to apportion upstream emissions under a flat carbon penalty p_t, i.e., a carbon tax policy regime, at varying levels of the penalty, p_t, from \$20 to \$50 per tonne CO_2. The range of carbon penalties was chosen based on an initiative to price carbon at the federal level in Canada which starts at \$20 per tonne of CO_2 in 2019 and expected to ratchet up to \$50 per tonne by 2022. We perform the analysis for a key entity in the pipeline supply chain, the TMPL, henceforth denoted as firm f.

The additional economic costs imposed on the firms in the supply chain by the various allocation schemes can be computed from their allocations provided in Table 1. In particular, at the baseline emission profile, f is allocated 17.087, 9.374, 2.947, and 3.429 kt CO_2eq/day by the TUR, adjusted TUR, nucleolus, and Shapley mechanisms, respectively. Firm welfare $\theta_f(x)$ (measured in 1000\$/day) delivered by an allocation x (expressed in kt CO_2eq/day) is obtained by comparing it with the economic costs associated with the baseline allocation mechanism, $\bar{x}$, $\theta_f(x) = p_t[\bar{x}_f - x_f]$. Therefore, while the TUR mechanism delivers the baseline firm welfare of zero, $\theta_f(\bar{x}) = 0$, the adjusted TUR mechanism has an associated firm welfare, $\theta_f(\bar{x}^\mu) = 7.713p_t$. The nucleolus mechanism provides $\theta_f(z) = 14.14p_t$, and the Shapley mechanism delivers $\theta_f(x^S) = 13.658p_t$.

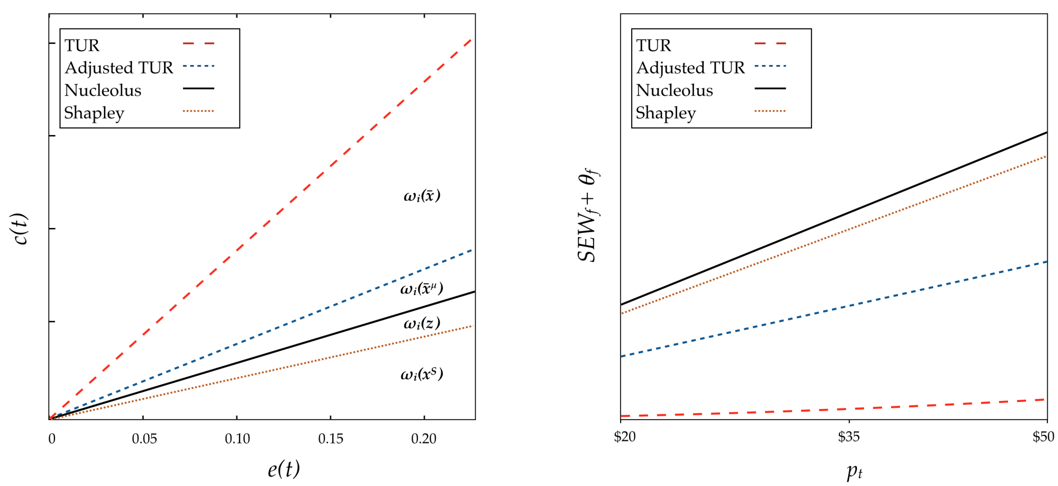


Figure 3.7: Region of potentially available technologies rendered profitable by the four allocation mechanisms (left panel). The social environmental welfare and firm welfare generated by the four mechanisms as a function of the carbon price, p_t (right panel).

To analyze the environmental effectiveness of each allocation mechanism, as discussed in §3.6, we evaluate $\omega_f(x)$, the area of the space of all potentially available costly emission-reduction technologies rendered profitable by each allocation mechanism. Recall that 0.227

is the direct emissions of f, and consider all potentially available technologies t with an associated emission reduction $0 < e(t) \leq 0.227$ at a cost $0 \leq c(t) < \infty$. Upon adopting technology t, the TUR allocation is given by, $\bar{x}_f(a_f - e(t); a_{-f}) = 17.087 - e(t)$, and the adjusted TUR by, $\bar{x}^{\mu}_f(a_f - e(t); a_{-f}) = (c(N) - e(t))(\bar{x}_f - e(t))/((\sum_{i\in N} \bar{x}_i) - 4e(t)) = (105.537 - e(t))(17.087 - e(t))/(192.38 - 4e(t))$. It can also be easily seen that the nucleolus alliance structure of the supply chain does not change by the adoption of emission reducing technologies by firm f, and therefore, $z_f(a_f - e(t); a_{-f}) = 2.947 - e(t)/3$. Further, since the Shapley mechanism attributes an equal share of the emissions a_f to each entity downstream to f, we have, $x^S_f(a_f - e(t); a_{-f}) = 3.429 - e(t)/4$. For an allocation x, we recall that $\omega_f(x)$ is the area of the region (denoted by $R_f(x)$), defined by $0 < e(t) \leq 0.227$ and $0 \leq c(t) < p_t[x_f(a_f; a_{-f}) - x_f(a_f - e(t); a_{-f})]$. In Figure 3.7 (left panel), we depict $\omega_f(x)$ for the four allocation mechanisms considered.

Further, we note that the social environmental welfare derived from the adoption of a technology t would be $p_t e(t) - c(t)$. Therefore, we denote by $SEW_f(x) = \int_{R_f(x)} (p_t e(t) - c(t))dt$, the total social environmental welfare associated with the incentives offered by an allocation mechanism x to adopt potentially available emission abatement technologies. We numerically evaluate the integral for the four different allocation mechanisms, and obtain the relative performances of the nucleolus allocation, $SEW_f(z)/SEW_f(\bar{x}^{\mu}) = 0.801$, $SEW_f(z)/SEW_f(\bar{x}) = 0.554$, and $SEW_f(z)/SEW_f(x^S) = 1.270$.

A comprehensive comparison of the allocation mechanisms would also incorporate the welfares delivered to the firm along with the social environmental welfare from incentivizing potentially available emission abatement technologies. Therefore, in Figure 3.7 (right panel), we plot $SEW_f + \theta_f$ as a function of the carbon price, p_t. We observe that the nucleolus mechanism outperforms the other three allocation mechanisms in terms of $SEW_f + \theta_f$ across p_t. In our example, this is driven by the substantially lower economic costs levied on the pipeline under the nucleolus mechanism resulting in higher firm-level welfare, $\theta_f(z)$. The nucleolus mechanism unambiguously outperforms the Shapley mechanism and generates higher firm-level welfare as well as incentivizes a larger set of potentially available emission abatement technologies. The nucleolus mechanism also performs fairly well in capturing the environmental benefits relative to the TUR, that allocates all upstream emissions to each individual firm, as reflected in our numerical estimates. We further note that while the inefficient baseline allocation mechanism, $\bar{x}$, shall always perform better than the nucleolus, z, at incentivizing potentially available emission abatement technologies, it is done at the expense of significantly lower supply chain and firm-level welfare.

In our example, the adjusted TUR mechanism performs marginally better than the nucleolus in terms of incentives offered, however, it delivers substantially lower firm welfare. Further numerical experiments, discussed in Appendix D, confirm that in supply chains where the baseline mechanism suffers from excessive double counting, that is, when μ is sufficiently large, the adjusted TUR mechanism performs worse than the nucleolus at incentivizing emission abatement technologies.

3.8. Discussion

The problem of assigning responsibility for emissions among the different members in extended supply chains has recently received attention in the environmental and life-cycle assessment literature (for example, Kander et al. 2015). Motivated by the Canadian federal government's guideline of factoring in upstream emissions during the environmental assessment of proposed energy projects, we adopt a natural cooperative game theoretic approach and propose the nucleolus of an associated cooperative game as a mechanism to apportion emission responsibilities while being concordant with the principle of upstream emission responsibility. Our contributions include (i) the development of a quadratic time algorithm to compute the nucleolus of the associated cooperative game, (ii) the clarification that in the context of fossil fuel supply chains, the nucleolus is the unique single-point game theoretic allocation mechanism with a natural consistency property. Such a property makes the nucleolus an especially desirable allocation method since fossil fuel supply chains typically span multiple legal jurisdictions. Further, and quite importantly, (iii) we provide a self-enforcing implementation framework consisting of easily-stated and compliance-verifiable policies, and a well-specified protocol, that are sufficient for the regulator to enforce the nucleolus mechanism to allocate upstream emissions in supply chains with profit-maximizing firms. We also, (iv) prove certain structural results that highlight the interpretability of the proposed nucleolus mechanism, (v) demonstrate that the nucleolus is the unique allocation mechanism that distributes the regulatory burden across the supply chain in a formalizably fair manner, and (vi) provide bounds on the welfare the nucleolus delivers to firms and its performance in terms of incentivizing firms to adopt potentially available emission reducing technologies.

Finally, we contextualize our results by analyzing a proposed pipeline project in Western Canada, the Trans Mountain pipeline expansion, that transports bitumen extracted from oil sands in Alberta to the ports of British Columbia. Our results illustrate the benefits and insights of the upstream responsibility principle, and more particularly, in adopting the nucleolus allocation mechanism in fossil fuel supply chains. We hope that they will serve as a useful case study for policy makers and environmental activists to analyze similar fossil fuel supply chains in other regions.

To assess the relative merits of our proposed nucleolus allocation mechanism, we could also consider the five evaluation criteria recommended by the Government of Canada, in 2005, to assess environmental tax proposals: (i) environmental effectiveness, (ii) fiscal impact,

(iii) economic efficiency, (iv) fairness, and (v) simplicity of administration. Adopting these as measuring sticks, we observe that the consistency property of the nucleolus mechanism, and its equilibrium properties subject to the easily stated and verifiable policies we provide, speak to the simplicity of administration and fairness. Fairness is also enshrined by the lexicographic distribution of welfares by the nucleolus allocation transposing the Rawlsian theory of justice to allocation problems as elaborated in §3.6. We also observe that the nucleolus allocation, by virtue of its footprint balancedness, is economically efficient under a carbon tax policy regime, as are all other footprint-balanced mechanisms. The fiscal impact of the nucleolus apportionment mechanism as well as its environmental effectiveness depend on the precise manner in which it is integrated with broader environmental policy regimes such as a carbon penalty. These are analyzed in §3.6, and in particular, in Theorems 3.6, 3.7, and 3.8, as well as in the case study.

Our results provide managerial implications for energy regulators. Indeed, they imply that a mandated, centrally determined and binding emission responsibility allocation scheme can be replaced, in some sense, by a decentralized scheme. That is, regulators can provide some degree of freedom to entities in fossil fuel supply chains to collectively arrive at an apportionment of pollution responsibilities that is beneficial from the entire supply chain's perspective. In that respect, it should be noted that a decentralized policy framework, that calls upon supply chain entities to collaborate with their partners, may catalyze additional ancillary environmental benefits.

Chapter 4

Bike-Sharing Systems: An Analysis of Operational Strategies

4.1. Introduction

Bicycle sharing is a transportation system in which bike stations are distributed across a region and users rent a bike for a short duration with the option of returning it at any other station. Bike sharing is fast emerging as a sustainable and environmentally friendly alternative, that complements the traditional modes of transportation to meet growing urban transport needs.

From an operational standpoint, bike sharing presents several unique challenges. Most notably, spatial asymmetries in the underlying demand, over time, results in certain stations with no bicycles to rent and some stations with no empty docks to return bikes. This necessitates rebalancing the stations periodically whereby bikes are relocated from stations that are full, to stations with zero or too few bikes. Efficient and frequent rebalancing has been observed to be crucial to the success of a bike-sharing program as it improves its reliability and has thus been the subject of extensive studies recently, for example, by Freund et al. (2019) and Raviv et al. (2013). Despite the growing popularity of bike sharing, systems in several major cities, such as Seattle's Pronto and Bixi in Montreal have run into financial difficulties. High operational costs arising from system rebalancing, theft and vandalism, coupled with lower than projected levels of ridership are commonly identified as the major contributing factors.

On the other hand, the environmental benefits of a bike-sharing program, as a consequence of reduced vehicular emissions from individuals substituting away from personal automobiles, might be less substantial than presumed. For example, the 2014 survey report of the Capital Bike Share Program in Washington D.C. notes that - "40% percent of respondents would have ridden a bus or train if Capital Bikeshare had not been available for the most recent trip, another 37% would have walked to their destination, only 12% of respondents would have driven or ridden in a car.” Another survey of bike-share users in Portland (PBOT 2016) estimated that only up to a quarter of the users had substituted away from cars. Further, typically the rebalancing operations are carried out with trucks which results in significant carbon emissions. Efficient rebalancing can therefore not only be economically desirable but could also potentially result in lower emissions from the rebalancing phase. Both these factors leads us to suggest that in certain cases, the environmental benefits of bike-sharing programs might be overstated. Lending further evidence, Fishman et al. (2014), using surveys and bike trip data, study the environmental impact of bike share programs across four cities world-wide, and find that the London bike-share system had a net negative environmental impact.

This motivates our work where we consider three key strategic and operational decisions faced by bike share operators - the coverage and density of the system, the pricing model and the frequency of rebalancing. Our objective is to develop a framework that can be employed by planners to design bike-sharing systems that are financially viable with high ridership and low operational costs which maximize environmental benefits.

Related Literature

In this work, we contribute and draw from three distinct strands of literature - the emerging operations literature on bike sharing programs, the growing field of sustainable operations management and the mature body of work pertaining to continuous approximation modelling of distribution problems.

Bike Sharing Programs. The sharing economy, and specifically, vehicle sharing business models, raise several challenging operational problems. Much of the existing literature on bike-sharing systems focuses on developing and solving optimization models to address specific operational problems during the management of these systems. Vehicle routing models for rebalancing bike stations efficiently have attracted much attention (see, for example, Raviv and Kolka 2013, Raviv et al. 2013, Shu et al. 2013, O’Mahony 2015, Freund et al. 2019, Schuijbroek et al. 2017). Another question of interest that has been studied pertains to the optimal allocation of docks across stations (O’Mahony 2015, Freund et al. 2017). In contrast, we adopt a holistic modelling approach that addresses the impacts of key operational strategic decisions undertaken by city planners while incorporating the role of existing modes of transport. In related work, Kabra et al. (2019) perform an empirical study to estimate the effects of accessibility and availability of bikes on ridership.

Continuous Approximation Modelling. Methodologically, we build on the continuous approximation (CA) modelling literature that develops analytical models to obtain qualitative insights on trade-offs in transportation systems. CA models, introduced by Newell (1973), provide an alternative to mathematical programming, i.e., discrete optimization models in the analysis of logistic systems. Unlike discrete optimization models that attempt to capture and model the system of interest as accurately as possible, CA models make approximate assumptions that replace discrete variables with continuous ones, in the interest of obtaining closed-form solutions. Along with analytical tractability, CA models also therefore allow the derivation of managerial insights. We refer the reader to Daganzo (2005) and Langevin et al. (1996) for a comprehensive discussion of the CA method and its application to logistics system analysis. Ansari et al. (2018) provide a more recent survey of CA applications. In the operations literature, CA models have also recently found applications in studies that provide high-level policy insights into the economic and environmental impacts of operational decisions in several settings such as retail location (Cachon 2014) and online grocery retail (Belavina et al. 2017). Our paper is most closely related to this line of literature.

Sustainable Business Models. More broadly, we also contribute to a growing sustainable business model innovation (Girotra and Netessine 2013) literature that studies the interactions between operational strategies and the economic and environmental performance of new business models, for example, shared logistics (Qi et al. 2018), online grocery retail (Belavina et al. 2016), and car sharing programs (Bellos et al. 2017).

4.2. Model Setup

We consider a region $\mathcal{R}$, such as a metropolitan area or a city, which either operates or is considering the adoption of a bike-sharing system. Unlike a majority of the operations literature on bike-share systems which assume an exogenous demand for each station, we model the underlying demand in the region $\mathcal{R}$ and assume an origin-destination transport demand function. The travel demand between any two locations u and v in the region, with a geographic distance between them denoted by $d(u, v)$ is given by $D(u, v)$. In this section, we describe the framework we adopt to model the operational and strategic decisions faced by the bike-share system operator, and the consumer utility model that governs the transport mode choice for different individuals.

4.2.1 Bike Share System Operator

We consider a transportation planner or an operator $\mathcal{O}$ who is planning to operate a bike sharing system in the region $\mathcal{R}$. The bike share system operator $\mathcal{O}$ faces several design considerations and operational decisions.

i. Coverage and Density. We assume that the operator $\mathcal{O}$ chooses a radius of coverage, R in which to locate the N bike share stations. By choosing a coverage radius, R, and given the number of stations, N, the operator consequently decides the density of stations per unit area, $\rho = N/\pi R^2$. This captures a fundamental strategic choice faced by bike-share operators of deciding between a sparse but widely spread system versus a smaller but denser system. We also note that in practice, as assumed in our model, typically the number of stations N is either an exogenous constraint on the operator or is a more stringent resource constraint.

We assume a fixed bike-sharing system wherein users rent bikes from stations at defined locations and return to any other station upon completion of the ride. This is a popular model in operation across many cities including Paris, New York and Vancouver. Alternately, $\mathcal{O}$ could also choose to operate a free-floating bike share system in which users find the closest bike to them via a mobile application and then could leave it at their destination. This eliminates the need for stations in the bike share system. Some bike share programs in China have adopted a free-floating model. We propose this as a potential extension of our model.

ii. Rebalancing Service Level. Spatial asymmetries in the underlying demand, over time, results in certain stations with no bicycles to rent and some stations with no empty docks to return bikes. This necessitates *rebalancing* the stations such that bikes are moved from stations with a more than optimal number of bikes to stations with zero or too few bikes. The operator $\mathcal{O}$ also chooses a rebalancing plan with an intent to maintain a specific service level, i.e., a specified probability ν of finding a bike (an empty dock) at a station. For example $\nu = 0.95$ would correspond to a situation wherein the probability of finding a bike (an empty dock) at a station is 0.95. Such service level requirements are routinely imposed on bike-share operators by the city and they, in turn, determine the extent of rebalancing that the operator will have to carry out.

iii. Pricing Model. A large majority of bike share systems adopt a subscription-based pricing model with an annual, monthly or a daily pass (or a combination of the three) with a fare which entitles pass holders to unlimited rides of a fixed duration T_B. Let the amortized fare averaged over the expected number of trips be denoted by K_B. Further, the user will incur a usage fee f_B per unit distance for rides exceeding the specified duration. A few bike share systems in Europe such as in Germany charge only the marginal usage fee. In this paper, we consider a unified framework for both pricing models by considering the marginal fee model as a case where $K_B = T_B = 0$ and model the subscription fee and the free-ride duration and the usage fee as set by the bike share operator $\mathcal{O}$. However, we recognize that in many instances the fare structure is also influenced by other considerations that are not necessarily revenue or welfare-maximizing, such as for example, to avoid competition with existing bike rentals.

4.2.2 Consumer's Mode Choice Model

We consider three distinct transport options - a private car (C), public transit (P) and bike-sharing (B). Further, we also consider the option of a bimodal transport option - that combines bike-sharing and public transit (BP). While we ignore other forms of transportation such as taxis and other emerging modes such as ride-sharing services for parsimony, our model can be extended to include these alternate modes of transportation without foregoing the key insights derived from our model and we leave this for future extensions of our model. We associate a utility function U_p^m for each mode of transport $m \in \{C, P, B, BP\}$ for every individual p in the population $\mathcal{P}$. We consider three drivers of mode choice behaviour.

i. Accessibility. Access time for mode m, τ_a^m is determined by the time to get from the individual's origin to the starting location of the service and getting from the end location of the service to the individual's destination. The access time for a privately owned vehicle is assumed to be zero.

ii. Service Level. Waiting time τ_w^m corresponds to the time spent in waiting to receive the service and is a measure of the service level of the system. For a privately owned vehicle, this is again reasonably assumed to be zero, while for a public transit option, it is tied to the frequency of the service. For bike sharing systems, while it is true that stations can be full or empty rendering them unavailable, most modern bike-sharing systems rely on mobile applications which convey the information on the availability of bikes and docks in neighbouring stations, thus essentially nulling the waiting time. However, it is to be noted that even in such systems with informative mobile applications, unavailability of bikes and docks in the closest station increases the access time of the system.

iii. Generalized Travel Cost. Generalized travel cost incorporates the travel fare τ_g^m for bike-share programs and public transit are determined by the monetary costs associated with the trip such as the fare or fuel cost, and the monetary equivalent of the in-vehicle travel time.

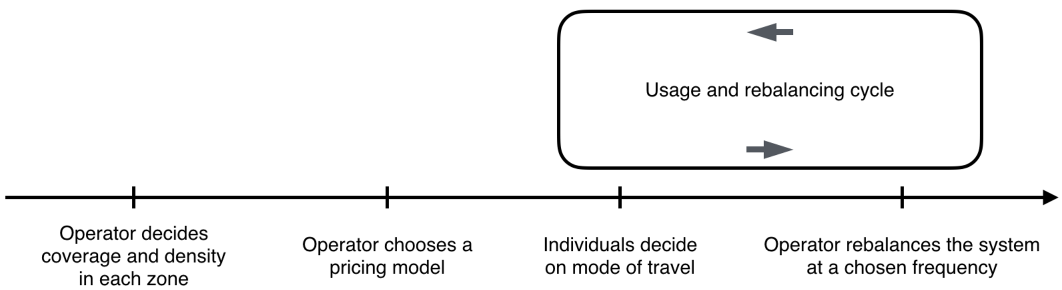
Note that we extend Kabra et al. (2016, 2019) who consider two main drivers of consumer demand in bike-share programs - availability and accessibility which correspond to our access time and waiting time. Traditionally, transportation models also incorporate factors such as income and age as explanatory variables in travel mode choice. We ignore these socio-economic factors in our model for mathematical tractability. However, we also note that these factors can be ignored by suitably choosing the population under consideration $\mathcal{P}$ as the set of individuals which are potential users of a bike sharing system. Indeed, several empirical studies have noted that users of bike share program typically are homogeneous in socio-economic characteristics.

The utility of a travel mode m for individual p with an origin-destination pair (u, v), consists of the utility that the individual derives from the trip, along with the disutility associated with the mode of transport associated with the drivers discussed previously,

$$U^m(p) = \theta(p) - \theta_a \tau_a^m(p) - \theta_w \tau_w^m(p) - \tau_g^m(p). \tag{4.1}$$

$\theta(p)$ denotes the intrinsic utility derived from the trip for an individual p with an origin u and a destination v. Note that equivalently, the utility function could alternatively be defined over trips with a given origin-destination pair (u, v), instead of over individuals. The utility derived for a trip with origin-destination given by (u, v) would be given by $U^m(u, v) = \theta(u, v) - \theta_a \tau_a^m(u, v) - \theta_w \tau_w^m(u, v) - \tau_g^m(u, v)$, where individuals have possibly different utilities for the trip, $\theta(u, v)$, drawn from a distribution F_{uv}.

Figure 4.1: Timeline of Events



Timeline of Events

The bike share program operator $\mathcal{O}$ initially chooses the radius of coverage. Subsequently, the operator decides on the pricing model of the program. Then, in each time period T, individuals of the population $\mathcal{P}$ evaluate the available modes of travel - private automobile, public transit, bike-share or a bimodal choice combining public transit and bike-share, and choose the utility-maximizing option considering travel time, accessibility, service level and travel fare. Also, periodically, during T, $\mathcal{O}$ rebalances the bikes in the system at a chosen frequency. The frequency of rebalancing operations, in turn, determines the service level of the bike-share system and therefore the usage of the system. The timeline of events is illustrated in Figure 4.1.

4.3. Operational Decisions and Bike-Sharing Demand

The operational decisions of the bike-share operator - the coverage of the system or equivalently, the density of stations and the rebalancing service level evidently affect the ridership in the system via their effects on the three drivers of mode choice. We thus begin our analysis by considering the impacts of these decisions on accessibility, service levels and generalized travel cost of the different travel mode options.

4.3.1 Drivers of Mode Choice

The access time of an individual to the bike-sharing program depends on the density of stations and the availability of *working* stations, that is, those that are neither empty nor full.

Theorem 4.1. (ACCESSIBILITY) *The average access time $\langle \tau_a^B \rangle$ for an individual using the bike-sharing system is given by,*

$$\langle \tau_a^B \rangle \cong \frac{4R\gamma\,(N,\nu)}{v_W}.$$

Theorem 4.1 provides an expression for the average access time for an individual using the bike-sharing system, where γ is a function of N and ν and further details are provided in the proof of Theorem 4.1. The access time for a private car is assumed to be zero, that is, $\tau_a^C = 0$, while the access time for public transit τ_a^P is exogenous to our model and reflects the density of existing public transit infrastructure in the city. For the bimodal option of using bike sharing and public transit for a trip, we have the access time $\tau_a^{BP} = \tau_a^B$. This is because, in the bimodal option, the individual uses bike-sharing to get to the public transit and therefore, the accessibility of the combined mode of travel corresponds to the accessibility of the first and last modes of transport which is bike-sharing.

The second driver of consumer travel mode choice relates to service levels of the corresponding modes, as measured by the time spent waiting to receive service, the waiting time. The waiting time for a private car is again assumed to be zero, that is, $\tau_w^C = 0$. The waiting time for a bike in a bike-sharing system is again zero because we have factored in the waiting time in the accessibility of the system. Indeed, recall that we defined the access time for an individual using bike-sharing as the time to the nearest available bike, and thus $\tau_w^B = 0$. The waiting time for public transit τ_w^P is exogenous to our model and corresponds to the frequency of existing transit operations in the region. For the bimodal option combining bike-sharing and public transit, the waiting time arises in the public transit phase of the option, and therefore, $\tau_w^{BP} = \tau_w^P$.

Now, we consider the third driver of mode choice - generalized travel cost. Generalized cost of travel comprises of both the fixed and variable monetary costs and the money-value corresponding to the travel time.

	Automobile	Public Transit	Bike Sharing	Bike Sharing – Transit
Access Time	$\tau_a^C = 0$	τ_a^P	τ_a^B (Theorem 4.1)	$\tau_a^{BP} = \tau_a^B$
Waiting Time	$\tau_w^C = 0$	τ_w^P	$\tau_w^B = 0$	$\tau_w^{BP} = \tau_w^P$
Generalized Travel Cost	τ_g^C (Remark 4.1)	τ_g^P (Remark 4.1)	τ_g^B (Remark 4.1)	τ_g^{BP} (Remark 4.2)

Table 4.1: Drivers of mode choice for the different modes of transport

Remark 4.1. *For an individual with origin u and destination v travelling by mode $m \in \{C, P, B\}$, the generalized cost of travel τ_g^m is given by $\tau_g^m = \left[\dfrac{d(u,v)}{v_m}\right]\theta_g + K_m + d(u,v)f_m$ where v_m, K_m, f_m correspond to the travel speed, fixed cost and marginal cost of mode m respectively.*

The fixed cost K_C for a trip with a private car corresponds to costs such as parking fees, while the variable cost f_C is the per-mile fuel cost. As mentioned earlier, K_B is the amortized fare averaged over the expected number of trips while f_B is the usage fee per unit distance for a bike-sharing program. While a large number of public-transit systems in North America operate on a flat rate or a zone-based fee structure, certain public transport systems have adopted a variable rate fare structure. Thus, we assume that K_P is the flat-rate for public transport in the region averaged over the expected number of trips while f_P denotes the variable fare rate. Further, let v_W denote the average walking speed of an individual.

Remark 4.2. *For an individual adopting the bimodal bike sharing and public transport option,*

$$\tau_g^{BP} = \left[\frac{d(u,v)}{v_P} + \frac{\tau_a^P v_W}{v_B}\right]\theta_g + K_P + K_B + \tau_a^P v_W f_B + d(u,v)f_P.$$

This is because, the in-vehicle travel time comprises of the time spent on the bike to cover the distances from the origin and destination to the nearest transit points, $\tau_a^P v_W$, in addition to the time spent in the public transit to travel the distance between the two transit points, which is on average $d(u,v)$. The public transit leg of the journey has a fixed cost K_P while the third term corresponds to the cost of using the bike-sharing program fee to get to and from the locations served by public transit. For individuals travelling from origin u to destination v, the costs corresponding to the three drivers of mode choice for each travel mode are summarized in Table 4.1 and the utility of using mode m of transport can thus be computed.

4.3.2 Transportation Mode Choice

Now, we are in a position to characterize the equilibrium transportation mode choices for individuals with different origin-destination pairs across the region and consequently, the equilibrium demand for the different modes of transport. We say that an individual p with an origin-destination pair (u,v) prefers mode a to mode b if p derives a larger utility from adopting mode a as opposed to mode b. For parsimony, we assume a deterministic mode choice model[1].

We assume that the speeds of the three modes of transport, v_C, v_P and v_B, are ordered such that $v_C > v_P > v_B$ and further that v_C is sufficiently greater than v_P which in turn is sufficiently greater than v_B[2]. Firstly, we consider the base situation when bike-sharing is not offered in the region. Then, in our model, a simple threshold exists to determine the choice between a private car and public transport.

Proposition 4.1. *An individual with origin-destination (u,v), prefers a car to public transport if and only if $d(u,v) > \tilde{d}_{CP}$ where,*

$$\tilde{d}_{CP} = \frac{K_C - K_P - \theta_a \tau_a^P - \theta_w \tau_w^P}{\theta_g \left[\frac{1}{v_P} - \frac{1}{v_C}\right] + f_P - f_C}.$$

We now consider the introduction of bike-sharing services in the region but without the possibility of the bimodal transport option. In Proposition 4.2, we identify threshold conditions on when the users prefer a car and public transport to using bike-sharing.

Proposition 4.2. *An individual with origin-destination (u,v), prefers a car to bike-sharing (respectively, public transit to bike-sharing) if and only if $d(u,v) > \tilde{d}_{CB}$ (respectively, $d(u,v) > \tilde{d}_{PB}$), where,*

$$\tilde{d}_{CB} = \frac{K_C - K_B - \frac{4R\theta_a\gamma(N,\nu)}{v_W}}{\theta_g \left[\frac{1}{v_B} - \frac{1}{v_C}\right] + f_B - f_C}, \tag{4.2}$$

$$\tilde{d}_{PB} = \frac{K_P - K_B + \theta_w \tau_w^P + \theta_a[\tau_a^P - \frac{4R\gamma(N,\nu)}{v_W}]}{\theta_g \left[\frac{1}{v_B} - \frac{1}{v_P}\right] + f_B - f_P}. \tag{4.3}$$

Further, we note that since bike-sharing systems have a finite radius of coverage, there will exist users who might prefer to adopt bike-sharing but are unable to do so because their origin or destination falls outside the coverage area. A continuous approximation lets us identify, given a coverage radius R, an upper bound for the travel distance $d(u,v)$ beyond

[1]The qualitative insights remain similar with other choice models such as a multinomial logit model and we leave this for an extension of our base model.

[2]The formal necessary condition is introduced in Appendix E.

which bike-sharing is not a viable mode of transport. We also refer the reader to Vaughan (1984) and Stone (1991) for similar results.

Lemma 4.1. *For a bike-sharing system with radius of coverage R, an individual with origin-destination (u, v) will not adopt bike-sharing if $d(u, v) \geq \widetilde{R}$, where $\widetilde{R} \cong \frac{32R}{9\pi}$.*

Finally, we now consider the bimodal option of bike-sharing with public transit. In Proposition 4.3, we provide conditions for when an individual prefers the bimodal option to each of the three other modes of transport, a car, public transit and bike-sharing.

Proposition 4.3. *Consider an individual p with origin-destination (u, v),*
i. p prefers the bimodal option to bike-sharing if and only if,

$$d(u,v) > \frac{\theta_w \tau_w^P + \tau_a^P v_W \left[\frac{\theta_g}{v_B} + f_B\right] + K_P}{\theta_g \left[\frac{1}{v_B} - \frac{1}{v_P}\right] + f_B - f_P} = \tilde{d}_{MB}, \tag{4.4}$$

ii. p prefers the bimodal option to public transit if and only if,

$$\theta_a(\tau_a^P - \tau_a^B) > \tau_a^P v_W \left(\frac{\theta_g}{v_B} + f_B\right) + K_B, \tag{4.5}$$

iii. p prefers the bimodal option to a car if and only if,

$$d(u,v) < \frac{K_C - K_B - K_P - \theta_a \tau_a^B - \theta_w \tau_w^P - \tau_a^P v_W \left[\frac{\theta_g}{v_B} + f_B\right]}{\theta_g \left[\frac{1}{v_P} - \frac{1}{v_C}\right] + f_P - f_C} = \tilde{d}_{MC}. \tag{4.6}$$

In Figure 4.2, we obtain schematic plots to illustrate Propositions 4.1-4.3. The parameter values assumed for the schematic plots approximately reflect realistic estimates. We refer the reader to Appendix E for further details. Figure 4.2 identifies the mode choice of individuals for varying trip distances. Broadly, our model implies individuals choose a car for larger distances while preferring public transport or bike sharing for trips of shorter distances. This highlights the importance of studying the substitution patterns between public transport and bike-sharing. Moreover, the bi-modal option bears relevance on the environmental impacts as well as the revenue from both bike-sharing and public transport. We provide below analytical expressions for the economic and environmental impacts of introducing bike-sharing in the region.

From Propositions 4.1-4.3, given an individual with an origin u and a destination v, the mode of transport with the least disutility, i.e. the most preferred mode, is uniquely determined. Let us denote the chosen mode of transport for an origin u and destination v by $m(u, v)$.

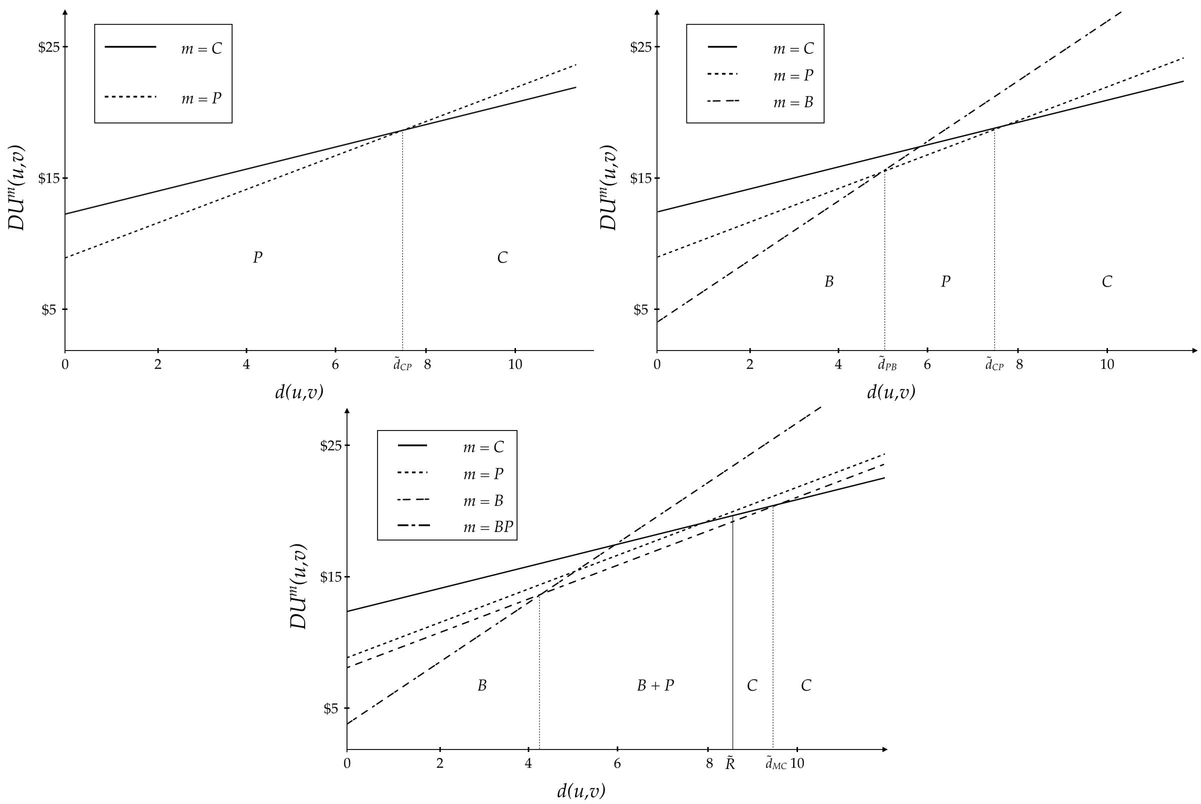


Figure 4.2: Disutilities of the various modes of transport and mode choice as a function of travel distance (units: km).

First, we quantify the economic impacts of bike-sharing. The revenue of the bike-sharing system, denoted by R_B, is given by,

$$R_B = \int\limits_{m(u,v)=B} (d(u,v) f_B + K_B) D(u,v) du dv \;\; + \int\limits_{m(u,v)=BP} (\tau_a^P v_W f_B + K_B) D(u,v) du dv. \quad (4.7)$$

That is, the revenue from bike-sharing arises from the per-unit distance fee and trip-averaged subscription fee paid by the individuals using bike-sharing for the entire trip as well as from individuals using bike-sharing as a mode of first and last-mile transport. Since it is important to also study the economic impacts of bike-sharing in the city on the public transit system, we need to compare the revenue of public transit with the revenue of public transit prior to the introduction of bike-sharing, denoted by R_P.

$$R_P = \int_{m(u,v)\in\{P,BP\}} (d(u,v)f_P + K_P)D(u,v)dudv \;\; - \int_{U^P(u,v)>U^C(u,v)} (d(u,v)f_P + K_P)D(u,v)dudv. \quad (4.8)$$

The change in revenue from public transit arises from individuals who earlier preferred a car over public transit but prefer to use the bi-modal option after the introduction of bike-sharing. In order to quantify the environmental impacts of bike-sharing, we need to analyze the patterns of mode substitution post the introduction of bike sharing in the region. We assume that public transit and bike-sharing are both non-polluting modes of transport, in that, they both generate zero usage emissions. We further assume that a car generates carbon emissions e_C per km and let p^S(\$/unit of emissions) denote the social cost of carbon. Then, the environmental benefits due to bike sharing in monetary terms is given by,

$$\Delta(E) = \int_{\substack{U^C(u,v)>U^P(u,v)\\ m(u,v)\in\{P,BP\}}} e_C d(u,v)D(u,v)dudv \;\; - e_T r(\nu). \quad (4.9)$$

In (4.9), $r(\nu)$ denotes the distance travelled by trucks during rebalancing operations to maintain a service level of ν. e_T denotes the carbon emissions generated by the trucks per km. In the next section, we provide a closed-form analytical expression for $r(\nu)$, thereby allowing us to perform numerical analyses to determine the economic and environmental impacts of various operational decisions undertaken by the bike-share operator.

4.4. Continuous Approximation for Bike Rebalancing Distance

A key logistical challenge for bike-share operators arises from spatial demand imbalances, that over time, result in some stations with too few or no bikes, and other stations which are full with no available docks to return bikes. Operators typically employ a fleet of trucks to rebalance the system periodically by moving bikes from surplus stations to deficit stations. The operational costs involved can be significant and finding optimal truck routes to perform the rebalancing operations aids in reducing these operational costs considerably. Efficient vehicle routing can also be beneficial from an environmental standpoint by helping achieve a lower carbon footprint. De Maio (2009) notes that rebalancing bikes from areas of high supply and low demand to areas with high demand and low supply is currently economically and environmentally expensive and flags this as an area for improvement in next-generation bike sharing systems.

The associated vehicle routing problem for bike-rebalancing is computationally hard (Erdogan et al. 2015) and has thus been a subject of extensive study. Hernández-Pérez et al. (2003) appear to be the first to consider the associated vehicle routing problem - the one-commodity pick-up and delivery travelling salesman problem. Exact algorithms (Erdogan et al. 2015), approximation algorithms with provable guarantees (O'Mahony et al. 2015) and heuristic approaches (Schuijbroek et al. 2017) have all been proposed to solve this problem. In this section, we eschew the numerical optimization approaches followed in the literature and instead adopt a continuous approximation method that allows us to obtain simple and useful guidelines for the associated truck routing problem and an estimate of the operational cost.

As before, we consider a bike-sharing system with N stations distributed over a coverage radius of R with a station density of $\rho = N/\pi R^2$. We assume the average spatial demand imbalance in the system to be distributed according to a Poisson distribution and denote the average spatial demand imbalance per unit time by λ. Therefore, λ denotes the average absolute difference between the in-flow and out-flow at each bike-sharing station. Further, suppose that the average capacity at each station is K bikes and K empty docks. The following result provides an expression for the average rebalancing distance covered by a truck to maintain a service level of ν across the bike-sharing system.

Theorem 4.2. *The average distance traveled to rebalance bikes across N stations, each with capacity K, distributed over a region with radius R and an average spatial demand imbalance rate of λ, is given by*

$$r(\nu, N, R, K, \lambda) \cong k_{TSP} f(\nu, K, \lambda) R\sqrt{\pi N}, \tag{4.10}$$

where $f(\nu, k, \lambda)$ is the rebalancing frequency required to maintain a service level of ν and is the solution to $Q\left(K+1, \lambda/f(\nu, K, \lambda)\right) = \nu$, where Q is the regularized gamma function[3].

The above expression for the rebalancing distance, $r(\nu, N, R, K, \lambda)$ comprises of two components. The first, $f(\nu, K, \lambda)$ refers to the number of rebalancing operations necessary to sustain a service level of ν. The second component, $k_{TSP} R\sqrt{\pi N}$, corresponds to the average distance traveled in each rebalancing stage. k_{TSP} is a scalar constant that is determined by the shape of the geographic region served, as well as the distance metric norm (i.e., L^1 or L^2 norms) employed[4].

In Figure 4.3, we provide a partial numerical confirmation of Theorem 4.2. Therein, we

[3] $Q(x, y) = \frac{\Gamma(x,y)}{\Gamma(x)}$, where $\Gamma(x, y) = \int_y^\infty t^{x-1} e^{-t} dx$ and $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dx$.

[4] We leave studying the effects of different geographic shapes and distance norms for an extension of our base model considered here.

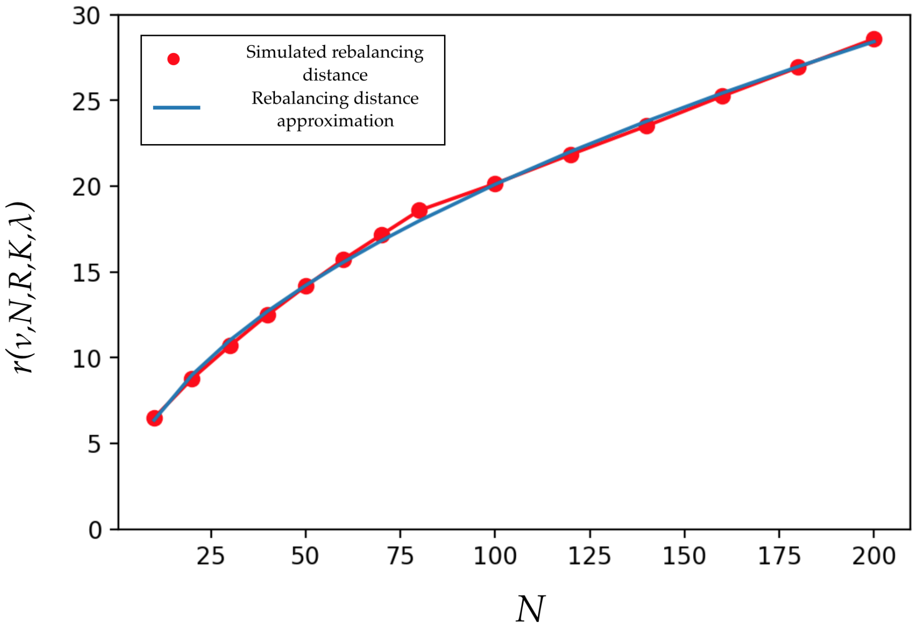


Figure 4.3: Comparison between approximation for $r(\nu, N, R, K, \lambda)$ from Theorem 4.2 and numerical estimates of rebalancing distance for simulated bike-sharing networks of different sizes N distributed over a region of unit-distance radius.

present the average rebalancing distance (with $f(\nu, K, \lambda)$ set to 1) for various simulated[5] bike-sharing networks of different sizes of N and compare it with the expression derived in Theorem 4.2. Figure 4.3 confirms that the rebalancing distance scales as $\sqrt{N}$.

4.5. Qualitative Implications and Extensions

From the numerical computations depicted in Figure 4.2, we obtain three salient observations. In the absence of the bi-modal (public transport and bike-sharing) option, bike-sharing substitutes exclusively away from public transport, thereby yielding no additional environmental benefits. This remains true for a wide range of parameter values. Thus, our model model findings are consistent with empirical reports from earlier studies such as Fishman et al. (2014) which observe high modal substitution to bike sharing from public transit (or simply walking). However, when we allow for the bi-modal option, the presence of a bike-

[5]All the simulations were carried out in Python 3.7. We generated 200 instances of N bike-sharing stations uniformly and randomly distributed over a region of radius 1 unit distance (for $N = 10, 20, 30, 40, 50, 60, 70, 80, 100, 120, 140, 160, 180, 200$). We then randomly initialized surplus and deficit stations (i.e stations with excess and fewer bikes, respectively, than the target level). The rebalancing distance for each instance was computed by employing a cluster-first and route-second heuristic to solve the associated TSP problem. A variation of the cluster-first route-second heuristic has been employed for the bike-rebalancing problem previously and shown to outperform other approaches (Schuijbroek et al. 2017).

sharing system generates positive environmental benefits by substituting certain car users to the bi-modal option. Further, it increases ridership, and equivalently revenues, of both bike-sharing and public transit. Finally, we also find in our numerical examples that the radius of coverage limits the uptake of bike-sharing, that is, $\tilde{d}_{MC} > \tilde{R}$. Individuals travelling between an origin-destination pair, (u, v), such that $\tilde{R} < d(u, v) \leq \tilde{d}_{MC}$ would have preferred to opt for the bi-modal option but are limited by the coverage of bike-sharing. Therefore, in certain situations, increasing the radius of coverage, even though it would result in lower density of bike-sharing stations, it might still result in higher net environmental benefits and greater revenues for bike-sharing and public transit. That is, the higher disutility due to an increase in the access time of bike-sharing is potentially outweighed by the increase in bi-modal demand from individuals who were previously unable to use the option due to limited bike-sharing coverage.

We suggest that the analytical expressions for the economic and environmental impacts of bike-sharing provided in equations (4.7)-(4.9) along with the expression for rebalancing distance developed in Theorem 4.2, can be employed to provide a theoretical confirmation of the preceding qualitative insights obtained via numerical analysis. Two other directions for future research are as follows. First, the robustness of our qualitative predictions can be tested by moving from the deterministic choice model described here to a stochastic mode-choice model (such as a multinomial logit model). This would allow us to empirically estimate and calibrate model parameters to real-world data. Finally, on that note, with the availability of bike-sharing data along with public transit and aggregate travel demand data, an empirical estimation and calibration of our model parameters will allow for more accurate and tailored qualitative recommendations.

To summarize, in this work, we have developed a transport modelling framework that incorporates key strategic and operational decisions faced by bike-sharing operators and city planners while introducing bike-sharing system to a city. It provides a pathway for the modelling framework developed herein to be employed by city planners to design bike-sharing systems that are financially viable with high ridership and low operational costs which maximize environmental benefits.

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Appendix A

Chapter 2 – Proofs and Technical Results

Proof of Proposition 2.1. Note that for $i \in N$ and $S \subseteq N$,

$$c_G(S \cup \{i\}) - c_G(S) = \sum \left(f_j : \text{ for all } j \in M \text{ such that } i \in N^j,\ S \cap N^j = \emptyset \right).$$

Clearly, for $Q \subseteq S$ and $j \in M$, if $S \cap N^j = \emptyset$ then $Q \cap N^j = \emptyset$. Therefore, for $i \in N$ and $Q \subseteq S \subseteq N$, $c_G(S \cup \{i\}) - c_G(S) \leq c_G(Q \cup \{i\}) - c_G(Q)$, which implies the concavity of (N, c_G). $\square$

Proof of Theorem 2.1. For each $j \in M$ and $S \subseteq N$, let $\left(N, c_G^j\right)$ denote the game where

$$c_G^j(S) = \begin{cases} 0, & \text{if } S \cap N^j = \emptyset, \\ a_j, & \text{otherwise.} \end{cases}$$

One can easily verify that for each $S \subseteq N$, $c_G(S) = \sum\limits_{j \in M} c_G^j(S)$. By its symmetry property, the Shapley value for the game $\left(N, c_G^j\right)$ is

$$\Phi_i^j = \begin{cases} \frac{f_j}{|N^j|}, & \text{if } i \in N^j, \\ 0, & \text{otherwise,} \end{cases}$$

and by its additivity property, $\Phi_i(c_G) = \sum\limits_{j \in M} \Phi_i^j$. Thus, the Shapley value of the GREEN game (N, c_G) allocates the cost of the pollution f_j equally among all players who can jointly influence the emissions at j. That is, for each process j, the Shapley value allocates f_j equally among all the firms in N^j. $\square$

Proof of Theorem 2.2. The set of maximizers of (2.4), $G(t)$, is a correspondence (a multi-valued function) from T to 2^X. A correspondence $G : T \mapsto 2^X$ is said to be a *concave* correspondence if for all t_1, t_2 in T, $x_1 \in G(t_1)$, $x_2 \in G(t_2)$, and $\lambda \in [0,1]$, there exists $x \in G(\lambda t_1 + (1-\lambda)t_2)$ with $x \geq \lambda x_1 + (1-\lambda)x_2$. From Theorem 5 of Jensen (2018), it follows that $G(t)$ is a concave correspondence in t. Finally, Lemma 2 of Jensen (2018) implies that the greatest selection of $G(t)$, $g(t) = \sup\ G(t)$, is also concave in t. □

Proof of Theorem 2.3. Let $\overline{BR}_i(x,t)$ denote the greatest best response for player i towards x_{-i} for parameter value $t \in T$. Then, $\overline{BR}_i(x,t) = \max\limits_{x_i \in X_i} u_i(x_i, x_{-i}, t)$ where $X_i \subset \mathbb{R}$. Denote $\widehat{T}_i = X_{-i} \times T$ and since $\widehat{T}$ is the product of two convex sets, it is also convex. Further, $u_i(x_i, x_{-i}, t) : X_i \times \widehat{T} \mapsto \mathbb{R}$ satisfies the quasi-concave differences property, that is, for all $\delta > 0$ in the neighbourhood of 0, $u_i(x_i, x_{-i}, t) - u_i(x_i - \delta, x_{-i}, t) = u_i(x_i, \hat{t}) - u_i(x_i - \delta, \hat{t})$ is quasi-concave in $(x_i, x_{-i}, t) = (x_i, \hat{t})$. Therefore, from Theorem 2.2, it follows that $\overline{BR}_i(x,t)$ is concave in $\hat{t} = (x_{-i}, t) \in \widehat{T}$. Therefore, for $t_1, t_2 \in T$, and $\alpha \in [0,1]$,

$$\begin{aligned}
\overline{BR}_i(\alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2), \alpha t_1 + (1-\alpha)t_2) &\geq \alpha\overline{BR}_i(\tilde{x}(t_1), t_1) + (1-\alpha)\overline{BR}_i(\tilde{x}(t_2), t_2) \\
&= \alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2),
\end{aligned}$$

where the equality holds since $\tilde{x}(t_1)$ and $\tilde{x}(t_2)$, by virtue of being equilibrium action vectors, are fixed points of the best-response function $\overline{BR}_i$ at t_1 and t_2, respectively. Further, since $\Gamma(t)$ is a supermodular game, Lemma 4.2.2 in Topkis (1998) implies that the best response $\overline{BR}_i(x,t)$ is increasing in the actions of the other players, $x_{-i} \in X_i$. Therefore, for $x > \alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2)$,

$$\begin{aligned}
\overline{BR}_i(x, \alpha t_1 + (1-\alpha)t_2) &\geq \overline{BR}_i(\alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2), \alpha t_1 + (1-\alpha)t_2) \\
&\geq \alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2).
\end{aligned}$$

Denote $\mathbb{1} = \sup X$, where $X \subseteq \mathbb{R}^n$ is a convex and compact set of all possible action vectors, with $n = |N|$ being the number of players in Γ. We obtain that, $\overline{BR}_i(\cdot, \alpha t_1 + (1-\alpha)t_2)$ maps $[\alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2), \mathbb{1}]$ into itself. From Brouwer's fixed point theorem, it then follows that $\overline{BR}_i(\cdot, \alpha t_1 + (1-\alpha)t_2)$ has a fixed point in the domain restricted to $[\alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2), \mathbb{1}]$. This fixed point, which will be an equilibrium of $\Gamma(\alpha t_1 + (1-\alpha)t_2)$ is greater than $\alpha\tilde{x}(t_1) + (1-\alpha)\tilde{x}(t_2)$ completing the proof of concavity of $\tilde{x}(t)$ in t. □

We now clarify the following technical lemma involving the composition of multi-dimensional concave functions, which we will subsequently employ in the proof of Theorem 2.4.

Lemma A.1. *Consider a sequence of functions, $\{h_i(x)\}_{i=1}^k$, where $x \in \mathbb{R}^n$, such that for all $1 \leq i \leq k$, $h_i : \mathbb{R}^n \mapsto \mathbb{R}$ is concave in x. Let $g : \mathbb{R}^k \mapsto \mathbb{R}$ be a component-wise convex decreasing function. Then, $\tilde{g}(x) = g(\{h_i(x)\}_{i=1}^k)$ is convex in x.*

Proof of Lemma A.1. Consider $x_1, x_2 \in \mathbb{R}^n$ and $\alpha \in [0,1]$. For all $1 \leq i \leq k$, the concavity of h_i implies,

$$h_i(\alpha x_1 + (1-\alpha)x_2) \;\geq\; \alpha h_i(x_1) + (1-\alpha)h_i(x_2).$$

Since g is decreasing, we have

$$\begin{aligned}\tilde{g}(\alpha x_1 + (1-\alpha)x_2) \;&=\; g(\{h_i(\alpha x_1 + (1-\alpha)x_2)\}_{i=1}^k)\\ &\leq\; g(\{\alpha h_i(x_1) + (1-\alpha)h_i(x_2)\}_{i=1}^k).\end{aligned}$$

From the component-wise convexity of g, we obtain,

$$g(\{\alpha h_i(x_1) + (1-\alpha)h_i(x_2)\}_{i=1}^k) \;\leq\; \alpha g(\{h_i(x_1)\}_{i=1}^k) + (1-\alpha)g(\{h_i(x_2)\}_{i=1}^k).$$

This implies that,

$$\tilde{g}(\alpha x_1 + (1-\alpha)x_2) \;\leq\; \alpha\tilde{g}(x_1) + (1-\alpha)\tilde{g}(x_2).$$

Therefore, $\tilde{g}(x) = g(\{h_i(x)\}_{i=1}^k)$ is convex in x. $\square$

Lemma A.2. *The equilibrium emission abatement effort vector, $\boldsymbol{e_j^\phi}$, for the decentralized first-stage game $\mathcal{G}(\phi)$, is concave in ϕ.*

Proof of Lemma A.2. From (2.5), the payoff function u_i for player i in $\mathcal{G}(\phi)$ is given by, $u_i = -\sum_{j\in\mathcal{P}_i} a_{ij}(e_{ij}) - \sum_{j\in\mathcal{P}_i} p^S\lambda_{ij}f_j(\boldsymbol{e_j}) = \sum_{j\in\mathcal{P}_i}\big(-a_{ij}(e_{ij}) - p^S\lambda_{ij}f_j(\boldsymbol{e_j})\big) = \sum_{j\in\mathcal{P}_i} u_i^j$. This allows us to decompose the game $\mathcal{G}(\phi)$ into a set of independent non-cooperative games, one for each process, $j \in M$, $\mathcal{G}^j(\phi)$. $\mathcal{G}^j(\phi)$ is supermodular since $f_j(\boldsymbol{e_j})$ is submodular. Further, the convexity of $\partial f_j/\partial e_{ij}$ and $\partial a_{ij}/\partial e_{ij}$ implies that u_i^j is concave in $(\boldsymbol{e_j}, \lambda_{ij})$. Then, from Lemma 1 of Jensen (2018), it follows that u_i^j exhibits quasi-concave differences. Therefore, the game $\mathcal{G}^j(\phi)$ is supermodular with the payoff function exhibiting quasi-concave differences, and a single-dimensional action set for each player. Therefore, Theorem 2.3 implies that the (greatest) equilibrium emission abatement vector $\boldsymbol{e_j^\phi}$, for the decentralized first-stage game $\mathcal{G}(\phi)$, is concave in ϕ. $\square$

Proof of Theorem 2.4. Consider any linear emission allocation rule ϕ, such that for a given firm i and process j, ϕ allocates the emissions $\lambda_{ij}f_j$ to firm i. Suppose that for the vector of cost functions $\boldsymbol{a} \in \mathcal{A}$, ϕ performs strictly better than the Shapley allocation rule, Φ, with respect to the equilibrium supply chain emissions. That is, $f^\phi(\boldsymbol{a}) < f^\Phi(\boldsymbol{a})$. We will show that there exists some permutation, $\boldsymbol{a'} \in \mathcal{A}$, of the functions in the cost function vector $\boldsymbol{a}$, at which $f^\Phi(\boldsymbol{a}) \leq f^\phi(\boldsymbol{a'})$. Note that this will complete the proof because it will contradict the existence of an allocation rule with a corresponding worst-case loss of efficiency being strictly smaller than the worst-case loss of efficiency corresponding to the Shapley value.

For each $j \in M$, consider an arbitrary permutation, π, of the vector of cost functions $\boldsymbol{a}_j = \{a_{ij} : i \in N^j\}$, resulting with the vector of cost functions $\boldsymbol{a}'_j$. That is, for any firm $i \in N^j$, $a'_{ij} = a_{\pi(i)j}$ for some $\pi(i) \in N^j$. The symmetry in efforts of the emission, f_j, of process j, implies that the effect of a permutation of the abatement cost functions on the equilibrium level of emissions is equivalent to the corresponding permutation of the share vector, from $\boldsymbol{\lambda}$ to $\boldsymbol{\lambda}'$, such that player $\pi(i)$, who originally was allocated the share $\lambda_{\pi(i)j}$, is now allocated $\lambda'_{\pi(i)j} = \lambda_{ij}$.

Note that for the Shapley allocation, the symmetry of the share vector implies that for any permutation of the cost functions, the equilibrium emission level remains the same, $f_j^{\Phi}(\boldsymbol{a}_j) = f_j^{\Phi}(\boldsymbol{a}'_j)$. For any other linear emission allocation ϕ, different from Φ, and for the permuted vector of cost functions, $\boldsymbol{a}'_j$, let $f_j(\boldsymbol{\lambda}')$ be the equilibrium emission level with $\boldsymbol{\lambda}'$ being the equivalent corresponding permutation of the share vector as described above.

From Lemma A.2, we have that equilibrium vector of abatement efforts, $\boldsymbol{e}_{\boldsymbol{j}}^{\phi}$, is concave in ϕ. Further, from Lemma A.1, it follows that $f_j(\boldsymbol{e}_{\boldsymbol{j}}^{\phi}(\boldsymbol{\lambda}')) = f_j(\boldsymbol{\lambda}')$ is convex in $\boldsymbol{\lambda}'$. Consider $\frac{1}{|N^j|!} \sum\limits_{\boldsymbol{\lambda}' \in \pi(\boldsymbol{\lambda})} f_j(\boldsymbol{\lambda}')$, where $\pi(\boldsymbol{\lambda})$ denotes all possible permutations of the share vector associated with f_j. The convexity of f_j in $\boldsymbol{\lambda}'$ and footprint balancedness, $\sum\limits_{i \in N^j} \lambda'_{ij} = 1$, implies that $\frac{1}{|N^j|!} \sum\limits_{\boldsymbol{\lambda}' \in \pi(\boldsymbol{\lambda})} f_j(\boldsymbol{\lambda}') \geq f_j\left(\frac{1}{|N^j|}, \frac{1}{|N^j|}, ..., \frac{1}{|N^j|}\right) = f_j^{\Phi}$. Thus, there exists some permutation $\boldsymbol{\lambda}'$ of the share vector $\boldsymbol{\lambda}$ such that the equilibrium emission level $f_j(\boldsymbol{\lambda}') \geq f_j^{\Phi}$.

Let the permutation $\boldsymbol{\lambda}'$ of the share vectors correspond to the permutation, $\boldsymbol{a}'_j$, of the abatement cost functions as described before. Then, equivalently, the equilibrium emission level with the vector of abatement costs given by $\boldsymbol{a}'_j$ at the allocation ϕ is given by $f_j^{\phi}(\boldsymbol{a}'_j) = f_j(\boldsymbol{\lambda}') \geq f_j^{\Phi}$. Repeating the same argument over all the processes proves that, in equilibrium, the allocation of $\frac{1}{|N^j|}$ of the pollution f_j to each firm in N^j, which is precisely the Shapley allocation, minimizes the worst-case loss of efficiency. □

We now present an alternate proof for a special case of Theorem 2.4. This alternate proof involves the repeated application of the implicit function theorem and therefore necessitates more restrictive assumptions on the footprint and abatement cost functions. This illustrates the usefulness of the generalized comparative statics tools developed in Section 2.4.1.

For each process j, the emission f_j, is assumed to be a symmetric decreasing convex function of the emission reduction efforts and, in addition, to be additive separable in the efforts by all firms, N^j, which are held responsible for the carbon footprint of process j. The additive separability assumption of carbon reduction efforts is made to perform the implicit function theorem analysis, and it is valid in several settings. For example, the design of a more efficient component by one supplier may not affect the emissions due to another component in the same product sourced from a different supplier. Further, several commonly assumed pollution abatement models in the literature satisfy the additive separable assumption.

The abatement cost functions $a_{ij}(e_{ij}) : [0,1] \to [0,A]$ are assumed to be convex and strictly increasing. For a process j, let $\boldsymbol{a_j}$ denote the vector of cost functions a_{ij} over all the firms $i \in N^j$ and let $\boldsymbol{a}$ denote the collective vector of cost functions over all the processes. Similarly, let $\boldsymbol{e_j}$ denote the vector of carbon reduction efforts by the firms in N^j and let $\boldsymbol{e}$ be the collective effort vector for all firms over all the processes. We also assume that f_j and c_{ij} have non-negative third derivatives for all firms i and processes j.

Alternate Proof of Theorem 2.4. Consider any linear emission allocation rule ϕ, such that for a given firm i and process j, ϕ allocates the emissions $\lambda_{ij} f_j$ to firm i. As before, suppose that for the vector of cost functions $\boldsymbol{a}_j$, ϕ performs strictly better than the Shapley allocation rule, Φ, with respect to the emissions at process j in equilibrium. We will show that there exists some permutation, $\boldsymbol{a}'_j$, of the functions in the cost function vector $\boldsymbol{a}^j$, at which $f_j^{\Phi}(\boldsymbol{a}_j) \leq f_j^{\phi}(\boldsymbol{a}'_j)$. This will complete the proof because it will contradict the existence of an allocation rule with a corresponding worst-case loss of efficiency.

The first-order condition for some player i who can influence the pollution at process j is given by $\dfrac{\partial a_{ij}(e_{ij})}{\partial e_{ij}} + p^S \lambda_{ij} \dfrac{\partial f_{ij}}{\partial e_{ij}} = 0$, where f_{ij} is the separable part of f_j due to the efforts of i. Applying the implicit function theorem, we obtain that $\left(p^S \lambda_{ij} \dfrac{\partial^2 f_{ij}}{\partial e_{ij}^2} + \dfrac{\partial^2 a_{ij}}{\partial e_{ij}^2}\right) \dfrac{\partial (e_{ij}^{\phi})}{\partial \lambda_{ij}} + p^S \dfrac{\partial f_{ij}}{\partial e_{ij}} = 0$. Note that $\dfrac{\partial f_{ij}}{\partial e_{ij}} < 0$ since f_{ij} is decreasing in e_{ij}. Also, $\dfrac{\partial^2 f_{ij}}{\partial e_{ij}^2} \geq 0$ and $\dfrac{\partial^2 a_{ij}}{\partial e_{ij}^2} \geq 0$ since f_{ij} and a_{ij} are convex in e_{ij}. Thus, $\dfrac{\partial (e_{ij}^{\phi})}{\partial \lambda_{ij}} > 0$ and therefore, we have that the equilibrium effort of i towards its pollution at process j, $e_{ij}^{\phi}(\lambda_{ij})$, is monotonically increasing in λ_{ij} (its allocated responsibility towards process j). Implicitly differentiating the first order condition a second time, we have,

$$\left(p^S \lambda_{ij} \frac{\partial^2 f_{ij}}{\partial e_{ij}^2} + \frac{\partial^2 a_{ij}}{\partial e_{ij}^2}\right) \frac{\partial^2 (e_{ij}^{\phi})}{\partial \lambda_{ij}^2} + 2p^S \frac{\partial^2 f_{ij}}{\partial e_{ij}^2} \frac{\partial e_{ij}^{\phi}}{\partial \lambda_{ij}} + \left(p^S \lambda_{ij} \frac{\partial^3 f_{ij}}{\partial e_{ij}^3} + \frac{\partial^3 a_{ij}}{\partial e_{ij}^3}\right) \left(\frac{\partial e_{ij}^{\phi}}{\partial \lambda_{ij}}\right)^2 = 0.$$

Further, noting the non-negativity of the third derivatives of f_{ij} and a_{ij} with respect to e_{ij}, and the convexity of f_{ij} and a_{ij} and that e_{ij}^{ϕ} is monotonically increasing in λ_{ij}, we conclude that,

$$\frac{\partial^2(e_{ij}^{\phi})}{\partial\lambda_{ij}^2} = -\frac{\left[2p^S\frac{\partial^2 f_{ij}}{\partial e_{ij}^2}\frac{\partial e_{ij}^{\phi}}{\partial\lambda_{ij}} + \left(p^S\lambda_{ij}\frac{\partial^3 f_{ij}}{\partial e_{ij}^3} + \frac{\partial^3 a_{ij}}{\partial e_{ij}^3}\right)\left(\frac{\partial e_{ij}^{\phi}}{\partial\lambda_{ij}}\right)^2\right]}{\left(p^S\lambda_{ij}\frac{\partial^2 f_{ij}}{\partial e_{ij}^2} + \frac{\partial^2 a_{ij}}{\partial e_{ij}^2}\right)} < 0.$$

Thus, we have that $e_{ij}^{\phi}(\lambda_{ij})$ is concave in λ_{ij}. The rest of the proof proceeds as before with appropriate notational modifications. □

Proof of Theorem 2.5. Consider process $j \in M$. From Lemma A.1 and Lemma A.2, as also observed previously, the equilibrium emissions at j, $f_j(\boldsymbol{e_j^{\phi}}) = f_j(\phi)$, is convex in the allocation vector, $\phi = \{\lambda_{ij} : i \in N^j\}$. Therefore, for the Shapley allocation vector, $\phi = \Phi$,

$$f_j^{\Phi} = f_j\left(\left[\frac{1}{|N^j|}\right]\right) \leq \frac{1}{|N^j|}f_j(\{\mathbf{1}\}) + \left(1 - \frac{1}{|N^j|}\right)f_j(\{\mathbf{0}\}),$$

where $\mathbf{0}$ and $\mathbf{1}$ denote the allocation vectors that assign to each firm in N^j zero and full responsibility for f_j respectively. Clearly, $f_j(\{\mathbf{1}\}) \leq f_j^*$ and $f_j(\{\mathbf{0}\}) = f_j^0$. Thus, $f_j^{\Phi} \leq \frac{f_j^*}{|N^j|} + \left(1 - \frac{1}{|N^j|}\right)f_j^0$. Rearranging,

$$f_j^{\Phi} - f_j^* \leq \left(\frac{1}{|N^j|} - 1\right)f_j^* + \left(1 - \frac{1}{|N^j|}\right)f_j^0 = \left(1 - \frac{1}{|N^j|}\right)(f_j^0 - f_j^*).$$

Summing over all $j \in M$,

$$f^{\Phi} - f^* \leq \left(1 - \frac{1}{\max|N^j|}\right)(f^0 - f^*).$$

Thus, we have,

$$\frac{\delta(\Phi, \boldsymbol{a})}{f^0 - f^*} = \frac{f^{\Phi} - f^*}{f^0 - f^*} \leq \left(1 - \frac{1}{\max|N^j|}\right).$$

This completes the proof. □

Proof of Theorem 2.6. Part i. The Shapley allocation rule is easily seen to satisfy the three properties. The proof of uniqueness is via induction. Consider the total pollution footprint $f = [f_1, f_2, ..., f_m]$ associated with the m processes, and let $f^0, f^1, ..., f^m$ be defined such that $f^0 = [0, 0, ..., 0]$, $f^1 = [f_1, 0, ..., 0]$ and so forth until $f^m = [f_1, f_2, ..., f_m] = f$. The proof is by induction. Clearly, any pollution allocation rule ϕ shall naturally allocate $[0, 0, ..., 0]$ to the firms in f^0 when all the processes have zero pollution. So, for f^0, $\phi(f^0) = \Phi(f^0)$, where Φ is the Shapley allocation rule. Let us assume that $\phi(f^{j-1}) = \Phi(f^{j-1})$, and we will prove that $\phi(f^j) = \Phi(f^j)$. For process j, let $|N^j| = n_j$. Define $\tilde{f}^j = (0, ..., 0, f_j, 0, ..., 0)$. For the footprint set $\tilde{f}^j$, by firm nullity any firm not in N^j must be allocated zero. By firm equivalence and efficiency, each firm in N^j is allocated $\frac{f_j}{n_j}$ when the pollution footprint set is $\tilde{f}^j$. Now, the pollution of process j alone increases by f_j in the footprint sets f^0 and f^{j-1} to yield $\tilde{f}^j$ and f^j, while the pollution of the other processes remains the same. For any firm $i \in N \backslash N^j$, $\phi_i(\tilde{f}^j) - \phi_i(f^0) = 0$ and for $i \in N^j$, $\phi_i(\tilde{f}^j) - \phi_i(f^0) = \frac{f_j}{n_j}$. Process history independence implies, $\phi_i(f^j) = \phi_i(f^{j-1})$ for $i \in N \backslash N^j$ and $\phi_i(f^j) = \phi_i(f^{j-1}) + \frac{f_j}{n_j}$ for $i \in N^j$. Thus, if $\phi(f^{j-1}) = \Phi(f^{j-1})$, $\phi(f^j)$ also has to be $\Phi(f^j)$, the Shapley allocation, and by induction, we conclude that $\phi = \Phi$.

We complete the proof by showing the independence of the three properties.

1. Consider the pollution allocation rule ϕ defined previously, that allocates to each firm the average pollution of all the processes, $\phi_i(f) = \frac{\sum_{j=1}^{m} f_j}{n}$. ϕ satisfies firm equivalence and process history independence but not firm nullity.

2. Consider a pollution allocation rule ϕ that allocates zero to each null firm, and shares equally the pollution among all the other firms. Such a rule naturally satisfies firm nullity and firm equivalence but in general it does not satisfy process history independence.

3. Consider again the pollution allocation rule that allocates the entire responsibility for each process to just one of the possibly many firms associated with it. It satisfies firm nullity and process history independence, but not firm equivalence.

Part ii. Again, it is easy to see that the Shapley allocation rule satisfies the three properties. Now, recall that firm i can influence the pollution at the set of processes, $\mathcal{P}_i$, and let $|\mathcal{P}_i| = m_i$. Consider a fully disaggregated supply chain derived as a result of each firm i in N disaggregating into m_i firms, each responsible for a distinct process in $\mathcal{P}_i$. In the fully disaggregated supply chain, each firm can now influence the pollution of at most one process. Following an argument similar to the one used in the proof for part (i), we have that firm-equivalence and no free riding imply that each firm in N^j is responsible for $\frac{f_j}{n_j}$. Invariance to disaggregation asserts that in the aggregated supply chain, each firm is responsible for the cumulative responsibilities of its disaggregated firms. This implies that again, the responsibility of each process is shared equally among the firms responsible for it, which is the Shapley allocation. We complete the proof by showing the independence of the three properties.

1. Consider a pollution allocation rule ϕ which allocates the pollution responsibility proportional to the individual responsibilities, $\phi_i(f) = \frac{f(\mathcal{P}_i)}{\sum_{k=1}^{n} f(\mathcal{P}_k)} \sum_{j=1}^{m} f_j$. This is similar to the responsibility allocation suggested by Lenzen et al. (2007) in order to obtain a disaggregation invariant allocation rule. While ϕ is disaggregation invariant and firm equivalent, it does not prevent free riding.

2. Let ϕ be a pollution allocation rule that allocates the pollution of each process equally

among some firms responsible for it and all other firms equivalent to it. ϕ is firm equivalent by definition, satisfies the no free riding property, but is not disaggregation invariant.

3. In the disaggregated supply chain, consider again the pollution allocation rule that allocates the entire responsibility for each process j to just one of the possibly many firms associated with it. In any aggregated supply chain, continue to allocate the responsibility of f_j to the possibly aggregated firm corresponding to the firm i that bears responsibility for j in the disaggregated supply chain. Such a pollution allocation rule is disaggregation invariant and prevents free riding. However, it is not firm equivalent. $\square$

Appendix B

Chapter 3 – Proofs and Technical Results

In this appendix, we develop technical results and subsequently employ them to provide proofs for results provided in the main text of the paper.

A. Preliminaries and Algorithmic Development

Consider the Upstream Responsibility game (N, c), with an associated directed tree $T = (V(T), E(T))$, as described in §3.2. Clearly, (N, c) is monotone.

Proposition B.1. *The Upstream Responsibility game (N, c) is concave.*

Proof of Proposition B.1. Note that for $i \in N$ and $S \subseteq N$,

$$c(S \cup \{i\}) - c(S) = \sum \left(e_k : e_k \in \mathcal{U}_i \backslash (\cup_{j \in S} \mathcal{U}_j)\right).$$

For $i \in N$ and $Q \subseteq S \subseteq N$, clearly if $e_k \in \mathcal{U}_i \backslash (\cup_{j \in S} \mathcal{U}_j)$, then, $e_k \in \mathcal{U}_i \backslash (\cup_{j \in Q} \mathcal{U}_j)$. Therefore, $c(S \cup \{i\}) - c(S) \leq c(Q \cup \{i\}) - c(Q)$, which implies the concavity of (N, c). $\square$

The concavity of the Upstream Responsibility game implies that it has a non-empty core (Shapley, 1971), the nucleolus allocation lies in the core (Schmeidler, 1969) and the nucleolus and pre-kernel coincide (Maschler et al., 1971). The monotonicity of the Upstream Responsibility game implies that all core solutions are non-negative.

Definition B.1. *A minimum excess coalition, S, $S \neq N$, with respect to an imputation x, which contains player i satisfies $c(S) - x(S) \leq c(T) - x(T)$, for all T containing i.*

Lemma B.1. *For a player i and a non-negative imputation x in the Upstream Responsibility game (N, c), there exists a minimum excess coalition containing i that includes all players in T_i.*

Proof of Lemma B.1. Let S be a coalition of minimum excess containing i and including the maximal number of players from T_i. Suppose there exists a $j \in T_i$ such that $j \notin S$.

Then, by definition of the characteristic function c, $c(S \cup \{j\}) = c(S)$. However, since x is non-negative, $x(S \cup \{j\}) = x(S) + x_j \geq x(S)$. Thus, $c(S \cup \{j\}) - x(S \cup \{j\}) \leq c(S) - x(S)$, contradicting the maximality of S. $\square$

Thus, by Lemma B.1, we can assume that a minimum excess coalition S containing player i also contains all players upstream to i.

Lemma B.2. *For players i and j in the Upstream Responsibility game (N, c), such that j is downstream to i, and a non-negative imputation x, $s_{ji}(x) = \min\{c(R) - x(R), j \in R, i \notin R\} = x_i$, and is achieved at $N \backslash \{i\}$.*

Proof of Lemma B.2. For such players i and j and $S \subset N$, $i \notin S$ and $j \in S$, $c(S) = c(S \cup \{i\}) \geq x(S \cup \{i\}) = x(S) + x_i$, implying $c(S) - x(S) \geq x_i$. Since $c(N \backslash \{i\}) - x(N \backslash \{i\}) = c(N) - x(N) + x_i = x_i$, the proof follows. $\square$

Lemma B.3. *Consider a pre-imputation z of the Upstream Responsibility game (N, c), that satisfies the following set of equations for each pair of adjacent players (i, j) in T, where j is the successor of i,*

$$\begin{cases} z_i = a(T_{ij}) - z(T_{ij}), \text{ if } z_j \geq a(T_{ij}) - z(T_{ij}), \\ z_i = z_j \text{ if } z_j \leq a(T_{ij}) - z(T_{ij}), \\ z(N) = c(N). \end{cases} \tag{B.1}$$

Then,
(I) For each pair of adjacent players i and j in T, $z_j \geq z_i$.
(II) The pre-imputation z is non-negative.

Proof of Lemma B.3. (I) follows trivially from the equations defining z. Consider (II); if $z_1 < 0$, then it follows from (I) that $z(N) < 0$, and since $c(N) \geq 0$, we obtained a contradiction to the assumption that z is a pre-imputation. Now, suppose that there exists some pair of adjacent players i and j such that $z_i < 0$ and $z_j \geq 0$. Then, by (I), $z_i = a(T_{ij}) - z(T_{ij})$. Now, from (I), $z_i \geq z_k$ for all $k \in T_{ij}$, and since $z_i < 0$, $z(T_{ij}) < 0$ as well. Therefore, $z_i = a(T_{ij}) - z(T_{ij}) > 0$, contradicting the assumption that $z_i < 0$, and we conclude that the pre-imputation z allocates non-negative cost shares to all players. $\square$

Proof of Theorem 3.1

First, we assume that z is the nucleolus of (N, c) and we will show that it satisfies (3.7). Since the nucleolus coincides with the pre-kernel in concave games, $s_{ij}(z) = s_{ji}(z)$ for adjacent players i and j, and since z is in the core, $z \geq 0$. Since j is a successor of i, it follows from Lemma B.2 that $s_{ji}(z) = z_i$. Now, suppose $s_{ij}(z) = min\{c(S) - x(S) : i \in S, j \notin S\}$ is attained at S^*, that is, $s_{ij}(z) = c(S^*) - x(S^*)$. If S^* contains a player on the path from j to the root, then $S^* = N \backslash \{j\}$. If S^* does not contain any player on the path from j to the root, then by Lemma B.1, S^* consists of all the nodes in T_{ij}. Thus, $z_i = s_{ij}(z) = min\{a(T_{ij}) - z(T_{ij}), z_j\}$, and we conclude that if z is the nucleolus, then it satisfies the set of equations in (3.7).

Now, suppose z is an allocation satisfying (3.7). For any two nodes k and l in the tree T, consider the unique paths from k and l to the root node, and let m be the first node in the paths common to both. By assumption, since only node 1 is adjacent to the root node, m is not the root node. Consider the sub-path, P, from k to m. Since z satisfies (3.7), it follows from Lemma B.3 that the allocation z is non-decreasing along P. Let r be the farthest node from k on P such that $z_r = z_k$. Note that since $a(T_r) - z(T_r) = z_r \leq z_i \leq a(T_i) - z(T_i)$, over all players $i \in P$, $a(T_i) - z(T_i)$ is minimized at $i = r$. Suppose $s_{k,l}(z)$ attains the minimum, $c(S) - z(S)$, at S^*, where $k \in S^*$ and $l \notin S^*$. Now, if S^* contains any firm downstream to l then, using the same proof technique as in Lemma B.2, we conclude that $s_{k,l}(z) = z_l$. If not, then $s_{k,l}(z) = a(T_r) - z(T_r) = z_r = z_k$. So, $s_{k,l}(z) = min(z_k, z_l)$. Similarly, $s_{l,k}(z) = min(z_l, z_k)$, and therefore $s_{k,l}(z) = s_{l,k}(z)$ for all pairs of players k and l. Thus, z is the pre-kernel and hence, since the Upstream Responsibility game (N, c) is concave, it coincides with the nucleolus. $\square$

Proof of Proposition 3.1

If player i resides in a leaf node, then by definition of the proto-nucleolus, $x_i = a_i - x_i$, implying that, $x_i = \frac{a_i}{2}$. We proceed via induction. Suppose (3.8) holds for all nodes which are upstream to player i. For adjacent players i and j with j being a successor of i, $x_i = a(T_{ij}) - x(T_{ij}) = a_i + \sum_{k \in U_i} (a(T_k) - x(T_k)) - x_i = a_i + \sum_{k \in U_i} x_k - x_i$, implying that $x_i = (a_i + \sum_{k \in U_i} x_k)/2$. For player 1 who has no successor player, since x is a preimputation, we have that $x_1 = a_1 + \sum_{k \in U_1} x_k$. $\square$

Proof of Proposition 3.2

Part i. If $x_i \leq x_j$ for all adjacent players i and j, then clearly the set of equations (3.8) characterizing the proto-nucleolus also satisfy the set of equations (3.7) in Theorem 3.1 that characterize the nucleolus. Therefore, the proto-nucleolus coincides with the nucleolus. The other direction is trivially true.

Part ii. Suppose $a(T_{ij}) \leq a_j$ for adjacent players i and j in the supply chain. Then, we claim that for all adjacent players i and j in the supply chain such that j is the immediate successor of i, $x_i \leq x_j$. If $j = 1$, from Proposition 3.1, $x_j = x_1 = a_1 + \sum_{i \in U_1} x_i$. Therefore, clearly, $x_j \geq x_i$

for $j = 1$ and $i \in U_1$. Suppose $j \neq 1$. Then, again from Proposition 3.1, $x_j = (a_j + \sum_{i \in U_j} x_i)/2$. Consider a firm $i \in U_j$ immediately upstream to j. Then, $x_j \geq (a_j + x_i)/2 = (a(T_{ij}) + x_i)/2 \geq (x_i + x_i)/2 = x_i$. The last inequality follows from the observation that the proto-nucleolus x is also a core allocation. Therefore, for all adjacent players i and j in the supply chain such that j is the immediate successor of i, $x_i \leq x_j$. Then, it follows from the proof of part (i) that the proto-nucleolus x coincides with the nucleolus z. □

Proof of Lemma 3.1

By Theorem 3.2, $z_j \leq z_1$ for each j. Therefore, since $z(N) = a(T)$, $z_1 \geq c_1$. Assume on the contrary, that there exists a player l, $l \neq 1$, for which $z_l < c_i$, and let k be a most downstream player for which $z_k < c_i$. By minimality of c_i, $z_k < c_k$. Thus, by Theorem 3.2, for all $j \in T_k$, $z_j \leq z_k < c_k$. Now, $\sum_{j \in T_k} z_j + (a(T_k) - z(T_k)) = a(T_k)$ and therefore, $a(T_k) - z(T_k) > a(T_k) - c_k|T_k| = a(T_k) - |T_k|a(T_k)/(|T_k|+1) = a(T_k)/(|T_k|+1) = c_k > z_k$. Let k' be the player immediately downstream to k. Then, $s_{k'k}(z) = z_k = s_{kk'}(z) = min(z_{k'}, a(T_k) - z(T_k))$, implying that, $z_k = z_{k'} < c_i$, which contradicts the assumption that k is a most downstream firm for which $z_k < c_i$. Thus, for all $j \in N$, $z_j \geq c_i$. Suppose now, on the contrary, that for some $j \in T_i$, $z_j > c_i$. Then, $z_i \geq z_j > c_i$. Since $\sum_{k \in T_i} z_k + (a(T_i) - z(T_i)) = a(T_i)$, it follows that, $a(T_i) - z(T_i) < a(T_i)/(|T_i|+1) = c_i$. Let i' denote the player immediately downstream to i. Then $s_{i'i}(z) = z_i = s_{ii'}(z) \leq a(T_i) - z(T_i) < c_i$, contradicting our previous conclusion that $z_i > c_i$. Thus, for all $l \in T_i$, $z_l = c_i$. □

Proof of Theorem 3.3

From Lemma 3.1, the nucleolus z allocates c_i to all players, N_i, in T_i, the first subtree generated in Step 1 of Algorithm A. Consider the reduced game $(\bar{N}_i, \hat{c}^z_{\bar{N}_i})$ on $\bar{N}_i = N \backslash N_i$ at z. The characteristic cost function $\hat{c}^z_{\bar{N}_i}(Q)$, $Q \subseteq \bar{N}_i$, of the reduced game $(\bar{N}_i, \hat{c}^z_{\bar{N}_i})$ of the Upstream Responsibility game (N, c) is given by $\hat{c}^z_{\bar{N}_i}(Q) = \min\{c(Q \cup R) - z(R) : R \subseteq (\bar{N}_i)^c\}$. Denote by $(\bar{N}_i, \tilde{c}^z_{\bar{N}_i})$ the upstream responsibility game induced by the subtree of T spanned by the set of vertices $\bar{N}_i$. That is, $(\bar{N}_i, \tilde{c}^z_{\bar{N}_i})$ is induced by the original tree graph wherefrom T_i and arc (i, j) were removed, where j is the immediate successor of i, and a_j was increased by $c_i = z_i = \frac{a(T_i)}{|T_i|+1}$. We will show that the reduced game $(\bar{N}_i, \hat{c}^z_{\bar{N}_i})$ coincides with $(\bar{N}_i, \tilde{c}^z_{\bar{N}_i})$.

Consider a coalition Q, $Q \subseteq \bar{N}_i$. If Q does not contain a node downstream to i (in the original tree T), then $\hat{c}^z_{\bar{N}_i}(Q) = \min\{c(Q \cup R) - z(R) : R \subseteq (\bar{N}_i)^c\} = \min\{c(Q) + c(R) - z(R) : R \subseteq (\bar{N}_i)^c\}$, and since $c(R) \geq z(R)$ for all $R \subseteq (\bar{N}_i)^c$, we conclude that $\hat{c}^z_{\bar{N}_i}(Q) = c(Q) = \tilde{c}^z_{\bar{N}_i}(Q)$. If on the other hand, Q contains a firm downstream to i, then $c(Q \cup R) = c(Q)$ for all $R \subseteq (\bar{N}_i)^c$, and thus, since z is a non-negative vector, $\hat{c}^z_{\bar{N}_i}(Q) = \min\{c(Q \cup R) - z(R) : R \subseteq (\bar{N}_i)^c\} = c(Q) - z(\bar{N}_i^c) = c(Q) - |T_i| \cdot \frac{a(T_i)}{|T_i|+1} = c(Q) + \frac{a(T_i)}{|T_i|+1} - a(T_i) = \tilde{c}^z_{\bar{N}_i}(Q)$, and we conclude that the games $(\bar{N}_i, \hat{c}^z_{\bar{N}_i})$ and $(\bar{N}_i, \tilde{c}^z_{\bar{N}_i})$ coincide. However, since the nucleolus is consistent, that is, it has the reduced game property, the nucleolus allocations to players in $(\bar{N}_i, \tilde{c}^z_{\bar{N}_i})$ coincide with the nucleolus allocations to these players in the original Upstream Responsibility game and the correctness of the algorithm follows by induction. Since each step in the algorithm takes linear time in $|N|$, and they repeat at most $|N|$ times before termination, we conclude that Algorithm A runs in quadratic time. $\square$

B. Implementation Framework and Stability Analysis

Proof of Proposition 3.3

Suppose i and j belong to the same alliance $A_k \in \mathcal{A}$, then policy $\mathcal{P}$ implies that i and j should bear equal responsibility. If $i \notin A_k$ and $j \in A_k$, then the remnant upstream responsibility for the players in alliance A_k is $a(T_i) - x^{\mathcal{A}}(T_i)$ and their direct responsibility is $a(A_k)$. According to policy $\mathcal{P}$, players in A_k should bear equal responsibility and are permitted to leave an equal share to a downstream alliance if one exists. Further, according to policy $\mathcal{M}$, monotonicity of responsibilities must be maintained. This implies that $x^{\mathcal{A}}_j \geq \max\left\{x^{\mathcal{A}}_i, \frac{a(A_k)+a(T_i)-x^{\mathcal{A}}(T_i)}{|A_k|+1}\right\}$ if $j \neq 1$ and $x^{\mathcal{A}}_j \geq \max\left\{x^{\mathcal{A}}_i, \frac{a(A_k)+a(T_i)-x^{\mathcal{A}}(T_i)}{|A_k|}\right\}$ if $j = 1$. The proposition now follows from the assumption that all the players in the supply chain are rational. $\square$

Proof of Proposition 3.4

Suppose, on the contrary, that not all the firms in M_k are allocated identical responsibilities. Choose $Q \in M_k$ as a largest subset of firms in M_k that are all allocated identical responsibilities. The minimality of M_k implies that Q is not a minimal non-blocking set of firms. Therefore, by definition, there exists some alliance Q' in $\mathcal{A}$, whose members are in $N \backslash Q$, that either blocks Q or is blocked by Q. If Q' blocks Q, then, there exists firms $u_1, u_2 \in Q$ and $u'_1, u'_2 \in Q'$ such that u'_1 is upstream to u_1 and u'_2 is downstream to u_2. Policies $\mathcal{M}$ and $\mathcal{P}$ then imply that $x(u'_1) \leq x(u_1) = x(u_2) \leq x(u'_2)$. Therefore, the firms in Q' are also allocated the same responsibilities as the firms in Q. Since M_k is a minimal non-blocking set of firms and Q belongs to M_k, Q' must also belong to M_k, thereby contradicting the maximality of Q. Therefore, for all firms i and j in M_k, $x_i = x_j$.

Now, analogous to the set of equations (3.9), it follows from policy $\mathcal{P}$ that the players in M_k should bear responsibility for at least the remnant upstream emissions transferred to them by an upstream alliance, if such an alliance exists, which is equal to the allocation of any member in such an upstream alliance. Further, according to policy $\mathcal{M}$, monotonicity of responsibilities must be maintained. Therefore, for $j \in M_k$ and for any upstream firm $i \in U(M_k)$, $x^{\mathcal{A}}_j \geq \max\left\{x^{\mathcal{A}}_i, \frac{c(M_k)-x^{\mathcal{A}}(U(M_k))}{|M_k|+1}\right\}$ if $1 \notin M_k$, and $x^{\mathcal{A}}_j \geq \max\left\{x^{\mathcal{A}}_i, \frac{c(M_k)-x^{\mathcal{A}}(U(M_k))}{|M_k|}\right\}$ if $1 \in M_k$. The equalities in (3.11) follow from the assumption that all the players in the supply chain are rational. $\square$

Proof of Theorem 3.4

Consider the following requirements we place on the strategies of the players in Γ. For a nucleolus alliance structure $\mathcal{A}^n$, (i) player j offers an upstream player i to join j's existing alliance if i and j belong to the same alliance in $\mathcal{A}^n$, (ii) player j can either offer or not offer player i to join j's existing alliance if i and j do not belong to the same alliance in $\mathcal{A}^n$, (iii) player i accepts j's offer if and only if i and j belong to the same alliance in $\mathcal{A}^n$ and rejects otherwise. We claim that the above requirements, (i)-(iii), characterize the equilibrium path actions, $\pi(\tilde{\sigma})$, of the firms in any subgame perfect equilibrium (SPE) strategy profile $\tilde{\sigma}$ of the alliance formation game Γ. Clearly, any strategy profile σ that satisfies (i)-(iii) will generate the nucleolus alliance structure, $\mathcal{A}^n$. That is, $\mathcal{A}(\sigma) = \mathcal{A}^n = \{A_1^n, ..., A_m^n\}$, and let z_i denote the nucleolus allocation to player i.

Now, let us assume, without loss of generality, that the alliance A_k^n corresponding to subtree T_k^n was obtained in the k^{th} iteration of Algorithm A. The proof proceeds with a bi-level induction, firstly on the subtrees obtained in each iteration of the algorithm, and secondly, a backward induction on the players in the corresponding subtrees. Let $\tilde{\sigma}$ be an arbitrary SPE of Γ generating the corresponding alliance structure, $\mathcal{A}(\tilde{\sigma})$.

Base Case: T_1^n is the subtree obtained in the first iteration of Algorithm A. For each player $i \in T_1^n$, consider the subgame Γ_t with history H_t such that the player to take the next action is $i = n(H_t)$, and all preceding actions in $A(H_t)$ by players in T_1^n satisfy (i)-(iii). Note that we make no assumption on the actions of players not in T_1^n. Suppose i is the last leaf node in T_1^n that did not take any action. Then, we can assume that the immediate preceding move in Γ_t was the one where its downstream partner j offered i to join its alliance. If i accepts the offer, the alliance A_1^n is formed. If, according to $\tilde{\sigma}$, i rejects the offer, then i forms an independent alliance, $\{i\}$, and receives the allocation $x_i^{\mathcal{A}(\tilde{\sigma})}$. By the minimality of T_1^n, $x_i^{\mathcal{A}(\tilde{\sigma})} > z_i$. Therefore, it is optimal for i to accept j's offer and thus, i chooses an action that satisfies (i)-(iii). This case corresponds to the base case of the backward induction on the players in the subtree T_1^n. Now, suppose player i corresponds to a branch node in T_1^n, and suppose that in the preceding action, its downstream partner, j, offered i to join its alliance. If i accepts, then, since players in T_1^n satisfy (i)-(iii) in all preceding actions to i's action, it follows by the backward induction hypothesis that the succeeding players will also act in accordance with (i)-(iii), and the eventual alliance formed will be A_1^n. If, on the other hand, i rejects j's offer, then A_1^n will not form. Instead, an alliance A corresponding to some subtree of T_1^n will form such that either $i \in A$, or i is upstream to A. Again, $\mathcal{M}$ implies that the allocation i receives is at least as large as the allocation to a firm in A, and by the minimality of T_1^n, i will be worse off. Therefore, i will accept j's offer. Suppose now that by (i) - (iii), firm i should offer an upstream firm u to join its alliance. Then, if i offers u to join, by the backward induction hypothesis, u will accept the offer, and further the alliance A_1^n will form. If i does not offer u, then again, an upstream alliance A corresponding to some subtree of T_1^n will form, such that i is downstream to A, and similarly, i will receive a larger responsibility allocation by the minimality of T_1^n and $\mathcal{M}$. Finally, suppose i is the root node of T_1^n, and according to (i) - (iii), the current decision corresponds to i choosing to either accept or reject an offer by its downstream player $j, j \notin A_1^n$. Suppose player i accepts the offer, then i will either be part of, or downstream to an alliance that corresponds to a subtree of T distinct from T_1^n. Again, i will obtain a higher responsibility allocation and therefore, i should reject j's offer. Therefore, in any SPE $\tilde{\sigma}$, we have that all players in T_1^n will choose actions that satisfy (i)-(iii).

Induction Hypothesis: In any SPE strategy profile, $\tilde{\sigma}$, all players in alliances A_l^n, for $l = 1, ..., k-1$, created in the first $k-1$ iterations of Algorithm A will choose actions in accordance with (i)-(iii).

Inductive Step: We need to show that players belonging to alliance A_k^n will also choose actions in accordance with (i)-(iii). From the induction hypothesis, it is seen that irrespective of the actions of the players in A_k^n, the players in alliances A_l^n, for $l = 1, ..., k-1$, will choose actions that ensure the formation of their respective alliances. The proof for the inductive step then follows identically the proof for the base case, except that now the minimality of T_k^n in the k^{th} step of the iteration ensures that no player violates (i)-(iii) in a SPE, thus completing the induction.

Therefore, all players' actions in the supply chain will satisfy (i)-(iii), and thus, the corresponding alliance structure generated by $\tilde{\sigma}$, $\mathcal{A}(\tilde{\sigma}) = \mathcal{A}^n$. $\square$

The following technical result will be subsequently employed in the proof of Lemma 3.2.

Assertion B.1. *Consider a strong Nash-stable alliance structure $\mathcal{A}$. Then, there exists a strong Nash-stable alliance structure, $\mathcal{A}'$, satisfying the property that for $M_u, M_v \in M(\mathcal{A}')$, and $i \in M_u$, $j \in M_v$, if M_u is upstream to M_v, then $x_j^{\mathcal{A}'} > x_i^{\mathcal{A}'}$, and further, $x^{\mathcal{A}} = x^{\mathcal{A}'}$.*

Proof of Assertion B.1. Clearly, if $\mathcal{A}$ itself satisfies the above property, then $\mathcal{A}' = \mathcal{A}$. Suppose that $\mathcal{A}$ does not satisfy the property. This implies that there exists a minimal non-blocking set M_k such that for a minimal non-blocking set M_l that is immediately upstream to M_k, $x_j^{\mathcal{A}} = x_i^{\mathcal{A}}$ for $j \in M_k$ and $i \in M_l$. Consider M_k to be such a minimal non-blocking set that is most upstream. From Proposition 3.4, we therefore obtain that $x_j^{\mathcal{A}} = x_i^{\mathcal{A}} \geq \frac{c(M_k) - x^{\mathcal{A}}(U(M_k))}{|M_k|+1}$. Consider the alliance structure $\mathcal{A}'$ such that the alliances comprising M_l and the alliances comprising M_k are combined yielding $M_k \cup M_l$ as a minimal non-blocking set in $\mathcal{A}'$. Then, $c(M_k \cup M_l) = c(M_k)$, and $x^{\mathcal{A}'}(U(M_k \cup M_l)) = x^{\mathcal{A}}(U(M_k)) - x^{\mathcal{A}}(U(M_l))$. Now, in $\mathcal{A}'$, $i, j \in M_k \cup M_l$, and $x_j^{\mathcal{A}'} = x_i^{\mathcal{A}'} = \frac{c(M_k \cup M_l) - x^{\mathcal{A}'}(U(M_k \cup M_l))}{|M_k \cup M_l|+1} = \frac{c(M_k) - x^{\mathcal{A}}(U(M_k)) + x^{\mathcal{A}}(U(M_l))}{|M_k \cup M_l|+1} = \frac{c(M_k) - x^{\mathcal{A}}(U(M_k)) + x_j^{\mathcal{A}}|M_l|}{|M_k|+|M_l|+1} \leq x_j^{\mathcal{A}}$. The last inequality follows from the prior observation that $x_j^{\mathcal{A}} \geq \frac{c(M_k) - x^{\mathcal{A}}(U(M_k))}{|M_k|+1}$. The strong Nash-stability of $\mathcal{A}$ therefore implies that $x_j^{\mathcal{A}'} = x_j^{\mathcal{A}}$ and therefore, $x^{\mathcal{A}'} = x^{\mathcal{A}}$ preserving the strong Nash-stability. The above union operation can be repeated successively until the above property is satisfied for all pairs of minimal non-blocking sets and at each step, the strong Nash-stability shall be preserved as shown. This completes the proof. $\square$

Proof of Lemma 3.2

Consider the minimal non-blocking set structure of $\mathcal{A}$, $M(\mathcal{A})$. Suppose that $M(\mathcal{A})$ contains only contiguous sets of firms. We can then define an alliance structure $\mathcal{A}'$ such that each alliance in $\mathcal{A}'$ corresponds to some set $M_k \in M(\mathcal{A})$. That is, we consider the alliance structure $\mathcal{A}' = M(\mathcal{A})$. Clearly, $\mathcal{A}'$ is a contiguous alliance structure. Therefore, $M(\mathcal{A}') = \mathcal{A}' = M(\mathcal{A})$, which in turn implies, due to Corollary 3.1, that $x^{\mathcal{A}} = x^{\mathcal{A}'}$. Therefore, for the non-contiguous alliance structure $\mathcal{A}$, we have identified a contiguous alliance structure that results in an identical allocation of responsibilities and is therefore also strong Nash stable.

Moreover, we can assume that the alliance structure $\mathcal{A}$ satisfies the property described in Assertion B.1, since otherwise, as demonstrated in Assertion B.1, we can always transform $\mathcal{A}$ to satisfy the said property while yielding an identical allocation of responsibilities. Now, suppose that for some $M_k \in M(\mathcal{A})$, M_k is a non-contiguous set of firms in the supply chain. Let $M_k = \bigcup_{i=1}^{p} S_i$, where each S_i is a maximally contiguous set of firms in M_k. Assume, for brevity, that $1 \notin M_k$, since the same proof, with some natural modifications, can be applied for the case $1 \in M_k$. From Proposition 3.3, and since $\mathcal{A}$ is assumed to satisfy the property in Assertion B.1, for $j \in M_k$ and $i \in U(M_k)$, $x_j^{\mathcal{A}} = \frac{c(M_k)-x^{\mathcal{A}}(U(M_k))}{|M_k|+1} > x_i^{\mathcal{A}}$. Choose l such that $l = \arg\min_i \frac{c(S_i)-x^{\mathcal{A}}(U(S_i))}{|S_i|+1}$. Consider an alliance structure $\mathcal{A}'$ formed by a deviation by the firms in S_l to form a separate alliance. Then, the allocations to all the firms upstream to S_l remain identical and therefore, $x_j^{\mathcal{A}} > x_i^{\mathcal{A}'}$ for $j \in S_l$ and $i \in U(S_l)$.

Further, suppose, on the contrary, that $\frac{c(S_l)-x^{\mathcal{A}'}(U(S_l))}{|S_l|+1} \geq x_j^{\mathcal{A}}$. Then,

$$\frac{c(S_l)-x^{\mathcal{A}'}(U(S_l))}{|S_l|+1} = \frac{c(S_l)-x^{\mathcal{A}}(U(S_l))}{|S_l|+1} \geq x_j^{\mathcal{A}} = \frac{c(M_k)-x^{\mathcal{A}}(U(M_k))}{|M_k|+1} = \frac{\sum\limits_{i=1}^{p} c(S_i) - \sum\limits_{i=1}^{p} x^{\mathcal{A}}(U(S_i))}{\sum\limits_{i=1}^{p} |S_i|+1}.$$

From the first and last terms in the inequality chain, we obtain,

$$\frac{c(S_l)-x^{\mathcal{A}'}(U(S_l))}{|S_l|+1} \geq \frac{\sum\limits_{\substack{i=1\\ i\neq l}}^{p} c(S_i) - \sum\limits_{\substack{i=1\\ i\neq l}}^{p} x^{\mathcal{A}}(U(S_i))}{\sum\limits_{\substack{i=1\\ i\neq l}}^{p} |S_i|},$$

which implies that,

$$\frac{c(S_l)-x^{\mathcal{A}'}(U(S_l))}{|S_l|+1} \geq \min_{j\neq l} \frac{c(S_j)-x^{\mathcal{A}}(U(S_j))}{|S_j|} > \min_{j\neq l} \frac{c(S_j)-x^{\mathcal{A}}(U(S_j))}{|S_j|+1},$$

violating the minimality of S_l. Therefore, $\frac{c(S_l)-x^{\mathcal{A}'}(U(S_l))}{|S_l|+1} < x_j^{\mathcal{A}}$. However,

$$x_j^{\mathcal{A}'} = \max\left\{x_i^{\mathcal{A}'}, \frac{c(S_l)-x^{\mathcal{A}'}(U(S_l))}{|S_l|+1}\right\},$$

and both terms in the curly brackets were shown to be strictly smaller than $x_j^{\mathcal{A}}$. Therefore, if the firms in S_l deviate to form a separate alliance, resulting in the alliance structure $\mathcal{A}'$, they would be strictly better off. This violates the strong Nash-stability of $\mathcal{A}$. Therefore, there exists no such M_k that is non-contiguous in $\mathcal{A}$, which completes our proof. $\square$

Proof of Theorem 3.5

Consider the nucleolus alliance structure, $\mathcal{A}^n = \{A_k^n\}_{k=1}^m$, where each alliance, A_k^n, in $\mathcal{A}^n$ corresponds to the subtree T_k obtained in the k^{th} iteration of Algorithm A. Further, consider a contiguous alliance structure $\mathcal{A}$ such that $\mathcal{A} \neq \mathcal{A}^n$. We now show that $\mathcal{A}$ is not strong Nash stable. Let $1 \leq i \leq m$ be the smallest index for which the alliance $A_i^n \notin \mathcal{A}$. Consider the set of firms $S = A_i^n$. Since, all alliances A_k^n such that $1 \leq k < i$ are in $\mathcal{A}$, and $\mathcal{A}$ is contiguous, we obtain from Proposition 3.3, that the remnant upstream responsibility for S in the alliance structure $\mathcal{A}$ is identical as in the nucleolus alliance structure. Then, by the minimality of the subtree T_i, the set of firms S can profitably deviate to form the alliance A_i^n. Therefore, the alliance $\mathcal{A}$ is not strong Nash stable.

Now, we prove the strong Nash stability of $\mathcal{A}^n$. Suppose there exists a set of firms S that can profitably deviate from their existing coalitions. Let $\mathcal{A}$ be the alliance structure arising from the deviation of S from $\mathcal{A}^n$. Since the deviation is strictly profitable for S, it follows from Corollary 3.1 that $M(\mathcal{A}) \neq \mathcal{A}^n$. Further, from the proof of Lemma 3.2, we know that if S is a non-contiguous set of firms, then there exists a smaller contiguous set of firms $S' \subset S$ that could form a separate alliance and be strictly better off. Therefore, we can assume that S is itself contiguous. And since, S is contiguous and $\mathcal{A}$ is obtained by the deviation of S from $\mathcal{A}^n$, all the minimal non-blocking sets in $M(\mathcal{A})$ should also be contiguous. Let $1 \leq i \leq m$ denote the smallest index for which $S \cap A_i^n \neq \phi$. Consider the subgraph of T, $G_i = T \setminus \bigcup_{j=1}^{i-1} A_j^n$. There exists some k' such that $A_i^n = T_{k'}$, a subtree of G_i rooted at k'. Consider $M_l \in M(\mathcal{A})$ such that the alliance $S \subset M_l$. Clearly, $M_l \neq A_i^n$, because then S would have had to be a subset of A_i^n and then S would receive an identical allocation after the deviation contradicting the strict profitability of the deviation. Further, M_l is also a subgraph of G_i and either corresponds to a subtree $T_{l'} \neq T_{k'}$ rooted at l' or there exists some M_p that corresponds to the subtree $T_{l'}$ and is upstream to M_l. By the minimality of $A_{i'}^n = T_{k'}$, the allocation to the firms in $T_{l'}$ is greater than the allocation to the firms in $A_{i'}^n$, and further, therefore by policy $\mathcal{M}$, the firms in M_l (that includes the firms in S) are also all allocated an allocation greater than the allocation to the firms in $A_{i'}^n$. This implies that a deviation by S from the nucleolus alliance structure is not profitable for the firms in $S \cap A_{i'}^n \neq \phi$. This contradicts the assumption that S is a set of firms that can profitably deviate from their current coalitions.

Further, if $M(\mathcal{A}) = \mathcal{A}^n$, then $M(\mathcal{A}) = M(\mathcal{A}^n)$ since $\mathcal{A}^n$ is a contiguous alliance structure. The second part of the result then follows from Corollary 3.1 since if two alliance structures have identical minimal non-blocking set structures, then the induced responsibility allocations, $x^{\mathcal{A}}$ and $x^{\mathcal{A}^n} = z$, should also be identical. $\square$

C. Structural Properties

Proof of Proposition 3.5

Suppose, on the contrary, that there exists an alliance $A_1 \in \mathcal{A}^n$ such that $1 \in A_1$, but $A_1 \neq \{1\}$. Note that from Theorem 3.3, A_1 corresponds to a sub-tree T_1' obtained at the last iteration of Algorithm A. Let L denote the set of firms adjacent to player 1 in A_1, and consider $k \in L$ such that $k = \arg\min_{l \in L} a(T_l')/(|T_l'|+1)$, where T_l' is the subtree of T_1 rooted at l. By definition, $c_1 = a(T_1')/|T_1'| = (a_1 + \sum_{l\in L} a(T_l'))/(\sum_{l \in L} |T_l'| + 1) > \sum_{l\in L} a(T_l')/(\sum_{l\in L} |T_l'| + 1) \geq \sum_{l\in L} a(T_l')/\sum_{l\in L}(|T_l'|+1) \geq a(T_k')/(|T_k'|+1)$. This contradicts the minimality of c_1, and correspondingly, the existence of such a subtree T_1'. Therefore, there exists no such alliance A_1. This implies that a nucleolus alliance structure, $\mathcal{A}^n$, always contains the singleton alliance, $\{1\}$. $\square$

Proof of Proposition 3.6

Let (N, c) denote the corresponding Upstream Responsibility game and suppose that the direct emissions a_j of firm j increases by δ to $a_j + \delta$. Let us denote the corresponding modified cooperative game by (N, c'). Then, the characteristic cost function $c'(S) = c(S) + \delta$ for all $S \subseteq N$ such that there exists a firm in S downstream to j, and $c'(S) = c(S)$ if no such firm is present in S. We show that there exists $\Delta > 0$ such that for all $0 < \delta \leq \Delta$ and for all i, z_i is linear and non-decreasing in δ. This will complete the proof that the nucleolus allocation is piecewise linear and non-decreasing in the direct emissions of each firm in the supply chain.

For any subtree S of T, define $\kappa(S) = a(S)/(|S|+1)$. Further, define

$$\Delta = \min_{R,S \subseteq T, \kappa(S) \neq \kappa(R)} |\kappa(S) - \kappa(R)| > 0.$$

Denote by A_i the subtree obtained in the i^{th} iteration of Algorithm A applied to (N, c). Suppose there exists some index k such that for all $1 \leq i < k$, player $j \notin A_i$. Then, Algorithm A applied to (N, c') shall proceed as it does when applied to (N, c), until iteration $k-1$, and therefore the nucleolus allocation z' in the modified cooperative game (N, c') allocates an identical responsibility to the firms in $\bigcup_{i=1}^{k-1} A_i$ as it does in (N, c). Therefore, without loss of generality, we assume that $j \in A_1$. We first observe that given our choice of Δ, for all $\delta \leq \Delta$, the subtrees obtained from each iteration of the algorithm applied to (N, c) and (N, c') remain identical. This follows because, if $c_i = a(T_i)/(|T_i|+1) < c_j = a(T_j)/(|T_j|+1)$ where T_i and T_j are some sub-trees of T generated by Algorithm A to produce the nucleolus of (N, c). Then, in (N, c'), $c'_i \le (a(T_i) + \delta)/(|T_i| + 1) \le (a(T_i) + \Delta)/(|T_i| + 1) < a(T_j)/(|T_j| + 1) \le c'_j$. For firm $i \in A_1$, $z'_i = z_i + \delta/(|A_1| + 1)$ implying that z_i is linear and non-decreasing in δ.

Now, consider the upstream responsibility game induced by the subtree of T spanned by the set of vertices $\bar{N}_1 = N \backslash A_1$. That is, the game subsequent to the removal, by Algorithm A, of the players in A_1, wherein the pollution associated with arc (u, v), a_v, was increased by $\delta' \equiv \delta/(|A_1|+1) \equiv \alpha\delta$, u is the most downstream player in A_1 and v is its immediate successor in the original supply chain graph. Note that this reduced setting can be interpreted as an upstream responsibility game wherein the weight of an arc increases by $0 < \delta' = \alpha\delta < \Delta$. Thus, we can proceed inductively to show that all players either receive an identical allocation as in (N, c) or an allocation linearly increasing in δ', and therefore equivalently, linearly increasing in δ. Therefore, z_i is continuous piecewise linear and non-decreasing in the direct emissions of firm j, a_j. □

Proof of Proposition 3.7

Consider the direct emissions associated with firm j in the fossil fuel supply chain given by $a_j + \Delta$. Choose $\Delta > (|N| + 1)(\max_{i \in N} c(T_i))$. Clearly, Algorithm A will ensure that none of the firms in T_k, $k \in L$, will form an alliance with any of the firms in P_j, because such an alliance will also be responsible for Δ, and clearly $c(T_k)/(|T_k| + 1) < c(T_k) < \Delta/(|N| + 1) < c(A)/(|A|+1)$, where A is any alliance containing some firm in P_j. Therefore, for each $k \in L$, Algorithm A can be run independently on the subtrees $T_k \cup k'$, where k', as defined above, is the root node of the sub-supply chain with $k' \in P_j$ and adjacent to k. Further, the nucleolus allocation to the players in these sub-trees shall clearly not depend on Δ. Therefore, for sufficiently large Δ, $\frac{\partial z_i}{\partial \Delta} = 0$ where z_i is the nucleolus allocation to $i \in T_k,\ k \in L$.

Now, consider the remaining nodes in the supply chain. They correspond to the reduced supply chain consisting only of the firms in P_j and the root node, 1. We claim that $P_j \in \mathcal{A}^n$. Suppose, on the contrary, that upon applying Algorithm A on the reduced supply chain spanned by $P_j \cup \{1\}$, the alliance $\{P_j\}$ cannot be formed. That is, a sub-tree, P_m of $P_j \cup \{1\}$ is derived. By Proposition 3.5, $\{1\} \in \mathcal{A}^n$. Therefore, $P_m \subsetneq P_j$. Let the root nodes of P_j and P_m be u and v, respectively. Note that, $c_u = (a(P_j) + \Delta)/(|P_j| + 1)$ and $c_v = (a(P_m) + \Delta)/(|P_m| + 1)$, and by Algorithm A, since alliance $\{P_j\}$ cannot be formed, $c_v < c_u$. Observe that, $a(P_j)/(|P_j|+1) - a(P_m)/(|P_m|+1) \le a(P_j)/(|P_j|+1) \le \Delta/((|N|+1)(|P_j|+1)) < \Delta/((|P_j|)(|P_j| + 1)) = \Delta(1/(|P_j|) - 1/(|P_j| + 1)) \le \Delta(1/(|P_m| + 1) - 1/(|P_j| + 1))$. But this then implies that $c_u = (a(P_j) + \Delta)/(|P_j| + 1) < c_v = (a(P_m) + \Delta)/(|P_m| + 1)$, yielding a contradiction. Therefore, upon applying Algorithm A to the reduced supply chain, we obtain P_j as the minimal subtree in the subsequent iteration implying that $P_j \in \mathcal{A}^n$. Finally, from

Proposition 3.5, $\{1\} \in \mathcal{A}^n$. This completes our proof. $\square$

Proof of Proposition 3.8

Since A_k^n is an alliance belonging to a nucleolus alliance structure of the fossil fuel supply chain enterprise $\mathcal{SC}$, it follows from Theorem 3.3 that it is obtained in some iteration t of Algorithm A applied to the supply chain tree T. Suppose that u is the most downstream player in A_k^n. It also follows from Algorithm A, that each player in $V(T_u)\backslash A_k^n$ is in some alliance, in the alliance structure $\mathcal{A}^n$, and that every firm in these alliances is upstream to some members in A_k^n. Let us denote all these alliances of $\mathcal{A}^n$, by A_i^n, for $i \in U$. Let $\mathcal{SC}'$ denote the supply chain enterprise resulting from structural changes to $\mathcal{SC}$, none of which being upstream to any member of A_k^n. Suppose that each such alliance $A_i^n \in \mathcal{A}^n$, $i \in U$, also belongs to a nucleolus alliance structure, $\mathcal{A'}^n$, of the supply chain enterprise $\mathcal{SC}'$. Then, from Theorem 3.3, since any change is not upstream to some members of A_k^n, it follows that all these alliances A_i^n, $i \in U$, could be recovered in some iteration of Algorithm A applied to the supply chain tree T'. Observe that A_k^n will be a sub-tree in the reduced supply chain enterprise obtained subsequent to all the iterations that recovered the alliances A_i^n, $i \in U$. Therefore, since A_k^n is a feasible sub-tree in the optimization step of Algorithm A, it follows that the nucleolus allocation to the firms in A_k^n in the supply chain $\mathcal{SC}'$ is no greater than the allocation they would receive by being part of the alliance A_k^n of $\mathcal{A}^n$ corresponding to $\mathcal{SC}$.

Alternately, suppose that there exists some alliance $A_j^n \in \mathcal{A}^n$, $j \in U$, which is not part of any nucleolus alliance structure in $\mathcal{SC}'$. Note that the firms in A_j^n must be part of an alliance A' in $\mathcal{A'}^n$ corresponding to a connected subgraph of T' and further, this alliance should also include u. The latter follows from the observation that if the alliance does not include u, it would violate the correctness of Algorithm A applied to T, in the iteration which yielded the subtree corresponding to alliance A_j^n. Now, since the alliance A' includes the firms in A_j^n, as well as all the firms in A_k^n, the nucleolus allocation to the firms in A_k^n in T' is no greater than the nucleolus allocation to the firms in A_j^n in T. From Theorem 3.2, since the alliance A_j^n is upstream to A_k^n, the nucleolus allocation to the firms in alliance A_k^n in $\mathcal{SC}'$ is no greater than the nucleolus allocation to these firms in $\mathcal{SC}$. This completes the proof. $\square$

D. Fairness and Welfare Properties

Proof of Proposition 3.9

The proposed nucleolus mechanism induces non-negative welfares, since it belongs to the core of the game (N, c), and any core allocation x satisfies $\theta(S, x) = p_t(c(S) - x(S)) \geq 0$. Further, we observe that the welfare vector, $\Theta(S, x)$, is a scaling by p of the vector of excesses, $e(x)$, restricted to the set $S \subseteq N$. Therefore, the nucleolus mechanism also lexicographically maximizes $\Theta(S, x)$. Further, if the set S coincides with the set N, then it follows from the definition of the nucleolus that it is the unique mechanism that lexicographically maximizes $\Theta(N, x)$. $\square$

Proof of Theorem 3.6

a. For a firm i and given the nucleolus allocation z, $\theta_i(z) = p_t(\bar{x}_i - z_i)$. Suppose that i belongs to the alliance $A(i)$ in the nucleolus alliance structure derived by the application of Algorithm A on the supply chain with a baseline emission profile. Then, by the optimality of $A(i)$ in the corresponding iteration of Algorithm A, it follows that the allocation i would receive for being part of the alliance $A(i) \cap T_i$ is at least z_i. If i were part of the alliance $A(i) \cap T_i$, then, i would receive an allocation $x_i = \dfrac{\sum_{j \in T_i \setminus (A(i) \cap T_i)} \alpha_j a_j + a(A(i) \cap T_i)}{|A(i) \cap T_i| + \mathbb{I}_{i \neq 1}}$ for some $\alpha_j \leq 1$, $j \in T_i$. Therefore, $z_i \leq x_i \leq \dfrac{c\{i\}}{|A(i) \cap T_i| + \mathbb{I}_{i \neq 1}} = \dfrac{\bar{x}_i}{|A(i) \cap T_i| + \mathbb{I}_{i \neq 1}}$. Therefore, $\theta_i(z) \geq p_t\big(\bar{x}_i - \dfrac{\bar{x}_i}{|A(i) \cap T_i| + \mathbb{I}_{i \neq 1}}\big)$ yielding the first desired inequality.

Now, we provide a second approach to obtain lower bounds on the welfare gains delivered by the nucleolus allocation z. Suppose that $i = 1$, then 1 bears full responsibility for a_1 and since z must satisfy policy $\mathcal{P}$, it follows that 1 can at most be responsible for half of the emissions from each of the firms upstream to it. Therefore, $z_1 \leq a_1 + \dfrac{c(\{1\}) - a_1}{2}$, implying that, $\theta_i(z) = p_t(\bar{x}_1 - z_1) \geq p_t\Big(\dfrac{\bar{x}_i - a_1}{2}\Big)$.

If $i \neq 1$, then, it follows from above that, $z_i \leq x_i = \dfrac{\sum_{j \in T_i \setminus (A(i) \cap T_i)} \alpha_j a_j + a(A(i) \cap T_i)}{|A(i) \cap T_i| + 1} = \sum_{j \in V(T_i)} \beta_j a_j$. Note that, in fact, $\alpha_j \leq 1/2$, since each firm can pass on at most half of it's direct emissions downstream (which happens when it belongs to a singleton alliance). Therefore, for $j \in T_i \setminus (A(i) \cap T_i)$, $\beta_j \leq 1/4$. Further, if $|A(i) \cap T_i| = 1$, then i is the only firm in $A(i) \cap T_i$. Therefore, $\beta_i \leq 1/2$ and $\beta_j \leq 1/4$ for $j \in V(T_i)$ and $j \neq i$. If $|A(i) \cap T_i| = 2$, then, let firms i and j belong to $A(i) \cap T_i$. Then, $\beta_i = \beta_j = 1/3$, and $\beta_k \leq 1/4$ for $k \in V(T_i) \setminus \{i, j\}$. Finally, if $|A(i) \cap T_i| \geq 3$, then, $\beta_j \leq 1/4$, for all $j \in V(T_i)$. It follows that, in all situations, $\beta_i \leq 1/2$, and for at most one j that must be an immediate upstream partner of i, $\beta_j \leq 1/3$, while $\beta_k \leq 1/4$ for all other $k \in V(T_i) \setminus \{i, j\}$. Therefore, $z_i \leq \dfrac{a_i}{2} + \dfrac{\max_{j \in U_i} a_j}{3} + \dfrac{\sum_{k \in V(T_i) \setminus \{i,j\}} a_k}{4}$, implying that, $\theta_i(z) = p_t(\bar{x}_i - z_i) \geq p_t\left(\dfrac{3\bar{x}_i - a_i}{4} - \dfrac{\max_{j \in U_i} a_j}{12}\right)$. This completes our proof for the lower bounds on the welfare gains delivered by the nucleolus allocation mechanism.

b. Let a_i denote the associated BAU emissions for firm i. Consider a technology t, which upon adoption, will yield an emission reduction of e from the BAU emissions at firm i. Then, given an allocation mechanism x, the associated cost savings for firm i is given by $p_t(x(a_i; a_{-i}) - x(a_i - e; a_{-i}))$. Then, under $\bar{x}$, technology t will be profitable to adopt if and only if $c(t) \leq p_t e$. We note that $\bar{x}$ allows firm i to recover fully the economic benefits of technology t. Observe that $0 < e \leq a_i$, therefore, implying that $\omega_i(\bar{x}) = p_t a_i^2/2$.

Further, from Algorithm A, it follows that if firm i belongs to alliance $A(i)$, then it receives a share of at least $1/(|A(i)| + 1)$ of its own direct emissions according to the nucleolus allocation z_i. Upon adoption of technology t, $z_i = z(a_i - e; a_{-i})$, it follows, again from Algorithm A, that when the emissions attributed to i, a_i, reduces, the alliance that i is a part of in the nucleolus continues to lie within the set of firms in $U(A(i))$. Therefore, i shall be attributed at least $1/(|U(A(i))|+1)$ of its own direct emissions upon adopting t, implying that $c(t) \leq p_t e/(|U(A(i))|+1)$ is a sufficient condition for the adoption of technology t to be profitable under the nucleolus allocation. Thus, $\omega_i(z) \geq p_t a_i^2/2(|U(A(i))|+1)$, and we obtain that $1/(|U(A(i))|+1) \leq \omega_i(z)/\omega_i(\bar{x})$. Further, from Algorithm A, the nucleolus allocates at most $1/2$ the responsibility of a_i to firm $i \neq 1$, that occurs when i belongs to a singleton alliance. For $i = 1$, the nucleolus always allocates the full responsibility of a_i to i. Thus, $\omega_i(z)/\omega_i(\bar{x}) \leq 1/2$ for $i \neq 1$, and $\omega_i(z)/\omega_i(\bar{x}) = 1$, for $i = 1$. This completes our proof for the lower and upper bounds on the ability of the nucleolus to incentivize adoption of potentially available emission reduction technologies. □

Proof of Theorem 3.7

Consider the nucleolus alliance structure $\mathcal{A}^n$ for the fossil fuel supply chain represented by the directed tree T. From Algorithm A, and specifically, the proof of Proposition B.2, it follows that if $V(T) = \{1\} \bigcup\limits_{i \in U_1} V(T_i)$, then for any alliance $A^n \in \mathcal{A}^n$, all the firms in A^n belong exclusively to one of the $V(T_i)$'s, for $i \in U_1$. Indeed, such a decomposition implies that Algorithm A can be applied individually to each of the subtrees T_i to obtain the alliances in $\mathcal{A}^n$.

Consider a vector of technologies $\mathbf{t} = \{t_i\}_{i \in N} \in \mathcal{T}$, where t_i is a potentially available technology that can achieve an emission reduction of $e_i(t_i) \in (0, a_i]$ at firm i at a cost $c_i(t_i) \in [0, \infty)$. Suppose that, in equilibrium, $\mathbf{t}$ will be adopted by the supply chain, under a carbon price p_t and the baseline allocation mechanism $\bar{x}$. Then, for each $i \in N$, $\Delta_i^{\bar{x}}(\mathbf{t}) = p_t\bar{x}_i(a_i; a_{-i} - e_{-i}(t_{-i})) - p_t\bar{x}_i(a_i - e_i(t_i); a_{-i} - e_{-i}(t_{-i})) = p_t e_i(t_i) \geq c_i(t_i)$. Therefore,

$$\Omega(\bar{x}) = \int\limits_{\substack{\mathbf{t} \in \mathcal{T} \\ c_i(t_i) \leq p_t e_i(t_i)}} d\boldsymbol{t}, \tag{B.2}$$

Consider the nucleolus allocation z. From the decomposition property described above, when the direct emissions of firm i is reduced by $e_i(t_i)$, firm i shall continue to be in an alliance that lies exclusively in one of $V(T_i)$ for $i \in U_1$. Therefore, $\Delta_i^z(\mathbf{t}) \geq p_t e_i(t_i)/(1 + \max\limits_{i \in U_1} |T_i|)$. Then,

$$\Omega(z) \geq \int\limits_{\substack{\mathbf{t} \in \mathcal{T} \\ c_i(t_i) \leq \frac{p_t e_i(t_i)}{(1 + \max_{i \in U_1} |T_i|)}}} d\boldsymbol{t},$$

Therefore,

$$\Omega(z) \geq \frac{\Omega(\bar{x})}{(1 + \max_{i \in U_1} |T_i|)}.$$

This completes the proof. $\square$

Proof of Theorem 3.8

Part i. Suppose $T = S_k$. Consider i to be one of the k upstream firms in $N \setminus \{1\}$. Then, from Theorem 3.1 and the definition of the Shapley mechanism, it follows that x^S and z both allocate to firm i responsibility for half of its own direct emissions, $a_i/2$. Since both mechanisms are pre-imputations, it also follows that they also allocate identical responsibilities to firm 1. Since the two allocation mechanisms coincide, it follows that $\Omega(x^S) = \Omega(z) \leq \Omega(x^*)$. The last inequality follows since x^* is the socially optimal concordant mechanism.

Part ii. Suppose $a(T_{ij}) \leq a_j$ for all adjacent players $i, j \in N$. Then, from Proposition 3.2, the nucleolus z coincides with the proto-nucleolus and is characterized by equation (3.8). Therefore, the nucleolus allocation mechanism z attributes to each firm $i \neq 1$ in the supply chain responsibility for exactly 1/2 of its own direct emissions, a_i, as well as responsibility for a portion of upstream emissions. The Shapley mechanism, x^S, allocates responsibility to firm i for a fraction, $1/(|P_i| + 1)$ of its own emissions, a_i, where recall P_i denotes the set of firms in the fossil fuel supply chain lying on the unique path from firm i to the root node 1 including i but excluding 1. Consider a vector of technologies $\mathbf{t} = \{t_i\}_{i \in N} \in \mathcal{T}$, where t_i is a potentially available technology that can achieve an emission reduction of $e_i(t_i) \in (0, a_i]$ at firm i at a cost $c_i(t_i) \in [0, \infty)$. Suppose that, in equilibrium, $\mathbf{t}$ will be adopted by the supply chain, under a carbon price p_t and the Shapley mechanism x^S. Then, for each $i \in N$, $\Delta_i^{x^S}(\mathbf{t}) = p_t x_i^S(a_i; a_{-i} - e_{-i}(t_{-i})) - p_t x_i^S(a_i - e_i(t_i); a_{-i} - e_{-i}(t_{-i})) = p_t e_i(t_i)/(|P_i| + 1) \geq c_i(t_i)$. Therefore,

$$\Omega(x^S) = \int_{\substack{\mathbf{t} \in \mathcal{T} \\ c_i(t_i) \leq \frac{p_t e_i(t_i)}{|P_i|+1}}} d\boldsymbol{t}. \tag{B.3}$$

For the nucleolus allocation z, $\Delta_i^z(\mathbf{t}) \geq p_t e_i(t_i)/2$.
Then,

$$\Omega(z) \geq \int_{\substack{\mathbf{t} \in \mathcal{T} \\ c_i(t_i) \leq \frac{p_t e_i(t_i)}{2}}} d\boldsymbol{t},$$

Therefore,

$$\Omega(z) \geq \frac{(|P_i| + 1)\Omega(x^S)}{2} \geq \Omega(x^S).$$

The socially optimal concordant mechanism x^* in this case will coincide with the total producer responsibility allocation which allocates to each firm responsibility for only its own emissions a_i. It then follows by similar arguments that $\Omega(x^*) \geq \frac{\Omega(z)}{2}$. Therefore, if $a(T_{ij}) \leq a_j$ for all adjacent players $i, j \in N$, then $\Omega(x^S) \leq \Omega(z) < \Omega(x^*)$.

Part iii. From the proof of Proposition 3.7, it follows that for each $i \in N$, there exists a sufficiently large M which is a function of $\{a_{-i}\}$, such that if $a_i > M$, the nucleolus allocation z allocates responsibility to firm i for a fraction, $1/(|P_i| + 1)$ of its own emissions. Further, since, x^* should be concordant, it follows that for sufficiently large M, x^* should also allocate responsibility to firm i for a fraction, $1/(|P_i| + 1)$, of its own emissions. Since, otherwise, x^* would not satisfy concordance along the path P_i. Finally, the Shapley mechanism, as observed earlier, also allocates to firm i fraction, $1/(|P_i| + 1)$, of its own emissions.

Consider a technology, $\mathbf{t}^* = \{t_j^*\}_{j \in N} \in \mathcal{T}(x^*)$. Then, $\Delta_i^{x^*}(\mathbf{t}^*) = p_t x_i^*(a_i; a_{-i} - e_{-i}(t_{-i}^*)) - p_t x_i^*(a_i - e_i(t_i^*); a_{-i} - e_{-i}(t_{-i}^*)) = p_t e_i(t_i^*)/(|P_i| + 1) \geq c_i(t_i^*)$. Consider $\mathbf{t^S} = \mathbf{t^z} = \{t_i^*; t_j^0 : j \neq i \in N\}$ where t_j^0 denotes a null technology which yields zero emissions reduction at zero cost. As $a_i \to \infty$, $a_i - e_i(t_i^*) > M$, and since the three allocations allocate identical responsibilities to firm i for its own emissions, $\Delta_i^z(\mathbf{t^z}) = \Delta_i^{x^S}(\mathbf{t^S}) = p_t e_i(t_i^*)/(|P_i| + 1) \geq c_i(t_i^*)$. Further for $j \neq i$, clearly, the equilibrium condition is satisfied. Therefore, $\mathbf{t^S} \in \mathcal{T}(x^S)$ and $\mathbf{t^z} \in \mathcal{T}(z)$. Moreover, $a(\mathbf{t}^*) = \sum_{j \in N}(a_j - e_j(t_j^*)) = a_i - e_i(t_i^*) + \epsilon$ and $a(\mathbf{t^S}) = a(\mathbf{t^z}) = a_i - e_i(t_i^*) + \sum_{j \in N, j \neq i} a_j = a_i - e_i(t_i^*) + \epsilon'$. Therefore, it follows, that $\lim_{a_i \to \infty} a(\mathbf{t^S})/a(\mathbf{t}^*) = \lim_{a_i \to \infty} a(\mathbf{t^z})/a(\mathbf{t}^*) = 1$. $\square$

Appendix C

Chapter 3 – Carbon Footprinting Computations

Oil sands are deposits of bitumen, a dense oil that needs to be typically diluted with diluents to form diluted bitumen (dilbit) before transportation and refining. The planned dilbit capacity for the seven in-situ (IS) projects under consideration is 224,500 bbl/day (ECCC, 2016). A part of the diluted bitumen is also usually upgraded to synthetic crude oil (SCO), a lower density product variety, before transportation via pipelines. Due to the economic costs imposed by upgrading bitumen, and the increasing capability of refineries to refine dilbit, the growth in Canadian oil sands projection and the subsequent transportation via the pipeline is expected to largely consist of dilbit rather than SCO (OSM, 2017). Therefore, we restrict the scope of our analysis to the in-situ and diluted bitumen pathway (IS+B) rather than in-situ and upgrading (IS+Up).

We next compute the emissions associated with each stage of the fossil fuel supply chain associated with the Trans Mountain pipeline extension depicted in Figure 6.

A. Oil Sands Projects – Extraction Emissions

The seven mines under consideration were all found to extract bitumen using the steam-assisted gravity drainage (SAGD) method. ECCC (2016) provides the GHG emission factors during extraction and dilution phase of bitumen using the SAGD method as 75.1 kg CO_2eq/bbl for the year 2019 with minor variations moving ahead.

i. West Ells (Sunshine Oil)

The planned dilbit capacity for the West Ells mine operated by Sunshine Oil is 7,100 bbl/day. Assuming an emission factor of 75.1 kg CO_2eq/bbl, we obtain 0.533 kt CO_2eq/day.

ii. Vawn (Husky Energy)

The planned dilbit capacity for the Vawn mine operated by Husky Energy is 10,000 bbl/day. Multiplying with the appropriate emissions factor, we obtain a daily emissions of 0.751 kt CO_2eq/day.

iii. Edam East & West (Husky Energy)

The planned dilbit capacity for the West Ells mine operated by Husky Energy is 14,500 bbl/day. Multiplying with the appropriate emissions factor, we obtain 1.089 kt CO_2eq/day.

iv. Hangingstone Expansion (Japan Canada)

The planned dilbit capacity for the West Ells mine operated by Japan Canada is 28,600 bbl/day. Multiplying with the appropriate emissions factor, we obtain 2.148 kt CO_2eq/day.

v. Christina Lake Phase F (Cenovocus/ConocoPhillips)

The planned dilbit capacity for the West Ells mine operated by Cenovocus/ConocoPhillips is 71,400 bbl/day. Multiplying with the appropriate emissions factor, we obtain 5.362 kt CO_2eq/day.

vi. Foster Creek Phase G (Cenovocus/ConocoPhillips)

The planned dilbit capacity for the West Ells mine operated by Cenovocus/ConocoPhillips is 42,900 bbl/day. Multiplying with the appropriate emissions factor, we obtain 3.222 kt CO_2eq/day.

vii. Mackay River Phase I (Brion Energy)

The planned dilbit capacity for the West Ells mine operated by Brion Energy is 50,000 bbl/day. Multiplying with the appropriate emissions factor, we obtain 3.755 kt CO_2eq/day.

B. TMPL – Pipeline Emissions

From ECCC estimates, we obtain that the emission intensity of the pipeline is 6.0 kg CO_2eq/1000 tonne kilometres. This includes emissions associated with the pumping stations to transport the fuel as well as leakage emissions. The pipeline extends for a length of 1150 kilometres. Further, it transports 224,500 bbl/day of diluted bitumen from the seven projects. We need the density of the dilbit in order to estimate its tonnage. From the historical information about the density of Canadian dilbit blends obtained from Crude Monitor (http://www.crudemonitor.ca), we assume a density of 923.2 kg/m^3. A barrel corresponds to 158.98 litres, that is, 0.159 cubic metre. Thus, a barrel of dilbit weighs 146.79 kg, that is, 0.147 tonnes.

The associated pipeline emissions for TMPL becomes $0.147 \times 6 \times 224,500 \times 1150/10^9$ kt CO_2eq/day = 0.227 kt CO_2eq/day.

C. Westridge Terminal – Shipping Emissions

From ECCC (2016), the marine emissions associated with the pipeline expansion project is estimated to be 68 kt CO_2eq/year. Or, (68/365) kt CO_2eq/day = 0.186 kt CO_2eq/day.

D. Refining Emissions

Cai et al. (2015) provide an estimate of the greenhouse emissions of refineries in the United States processing bitumen from Canadian oil sands. We work with the assumption that these estimates are also reflective of the processing efficiency of refineries in the Asia-Pacific with an average associated GHG emissions of 13.4 g CO_2eq/MJ. A barrel of crude oil has an energy content of 6.1 GJ (Schmitz, 2011). Therefore, the refining emissions is estimated to be $(224,500 \times 6.1 \times 10^9 \times 13.4)$ kt CO_2eq/day/$(10^6 \times 10^9)$ = 18.350 kt CO_2eq/day.

E. Consumption Emissions

The refining efficiency from dilbit to gasoline is 84.8% (Cai et al., 2015), and the GHG emissions from burning a litre of gasoline(http://sustainableanalytics.ca/2017/07/04/gasoline-carbon-tax/) is 2.31 kg. Consumption emissions from the net dilbit is then, $0.848 \times 158.98 \times 224,500 \times 2.31$ kg CO_2eq/day = 69.914 kt CO_2eq/day.

Scope of Analysis

In this case study, we included those entities which are incorporated in the actual environmental impact assessment report of the TMPL (ECCC 2016). The report does not incorporate refineries or other stages downstream to the pipeline, but we have done so in order to provide as comprehensive an analysis as possible. We note that our cooperative game model and the subsequent analysis makes no assumptions as to which entities can or cannot be included in the supply chain under consideration. Further, typically, the scope of the evaluation process is clearly specified by the regulator. For example, the report specifies up front that the scope of the review does not extend to "indirect" upstream emissions generated during the production of inputs such as electricity or fuels, or the emissions generated from the transport of products from the oil sands to the TMPL. So, while determining the scope of the process is indeed critical from the perspective of the regulator and the firms in the supply chain, it does not in any way limit the application of our model.

Appendix D

Chapter 3 – Further Numerical Results

We now consider the following simple supply chain depicted in Figure 8. The weights on the arcs represent the baseline direct emissions of the corresponding entities. The subsequent numerical analysis is performed on firm 2 in the supply chain.

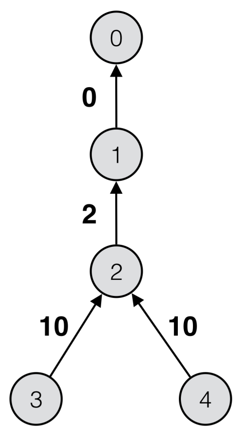

Figure D.1: A simple fossil fuel supply chain.

The TUR, adjusted TUR, nucleolus, and Shapley mechanisms for the supply chain can be easily computed along similar lines as in the case study presented in §3.7. Therefore, firm 2 is allocated 22, 7.5625, 6, and 7.6667 units by the TUR, adjusted TUR, nucleolus, and the Shapley mechanisms, respectively. Firm welfare $\theta_2(x)$ delivered by an allocation x is obtained by comparing it with the economic costs associated with the baseline allocation mechanism, $\bar{x}$, $\theta_2(x) = p_t[\bar{x}_2 - x_2]$. Therefore, while the TUR mechanism delivers the baseline firm welfare of zero, $\theta_2(\bar{x}) = 0$, the adjusted TUR mechanism has an associated firm welfare, $\theta_2(\bar{x}^{\mu}) = 14.4375p_t$. The nucleolus mechanism provides $\theta_2(z) = 16p_t$, and the Shapley mechanism delivers $\theta_2(x^S) = 14.3334p_t$.

To analyze the environmental effectiveness of each allocation mechanism, we evaluate

$\omega_2(x)$, the area of the space of all potentially available costly emission-reduction technologies to firm 2 rendered profitable by each allocation mechanism. Consider all potentially available technologies t with an associated emission reduction $0 < e(t) \leq 2$ at a cost $0 \leq c(t) < \infty$. Upon adopting technology t, the TUR allocation is given by, $\bar{x}_2(a_2 - e(t); a_{-2}) = 22 - e(t)$, and the adjusted TUR by, $\bar{x}_2^{\mu}(a_2 - e(t); a_{-2}) = (22 - e(t))^2/(64 - 2e(t))$. It can also be easily seen that the nucleolus alliance structure of the supply chain does not change by the adoption of emission reducing technologies by firm 2, and therefore, $z_2(a_2 - e(t); a_{-2}) = 6 - e(t)/2$. Further, since the Shapley mechanism attributes an equal share of the emissions a_2 to each entity downstream to 2, we have, $x_2^S(a_2 - e(t); a_{-2}) = 7.6667 - e(t)/2$. For an allocation x, we recall that $\omega_2(x)$ is the area of the region defined by $0 < e(t) \leq 2$ and $0 \leq c(t) < p_t[x_2(a_2; a_{-2}) - x_2(a_2 - e(t); a_{-2})]$. In Figure D.2 (left panel), we depict $\omega_2(x)$ for the four allocation mechanisms considered. In the right panel of Figure D.2, we plot $SEW_2 + \theta_2$ as a function of the carbon price, p_t computed as in §3.7.

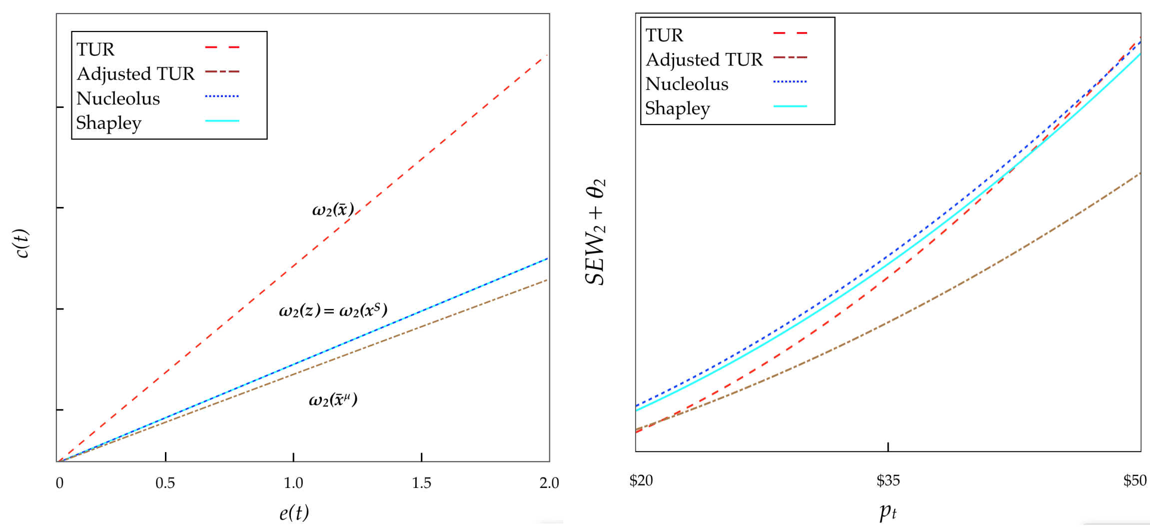

Figure D.2: Region of potentially available technologies rendered profitable by the four allocation mechanisms (left panel). The social environmental welfare and firm welfare generated by the four mechanisms as a function of the carbon price, p_t (right panel).

From Figure D.2 (left panel), we observe that, in this example, the nucleolus and the Shapley mechanisms perform identically with respect to incentivizing the adoption of potentially available emission reduction technologies. Further, both mechanisms outperform the adjusted TUR mechanism in this respect. Recall that in the case study, the adjusted TUR performed better than the nucleolus along this dimension. We reconcile this by observing that in the simple supply chain considered here, the extent of double counting, as measured by $\mu \approx 2.9$, is considerably higher than that in the case study, where it was, $\mu \approx 1.9$. This lends support to our observation that in supply chains with excessive double counting, the nucleolus mechanism will outperform the adjusted TUR with respect to incentivizing the adoption of potentially available emission reduction technologies.

Further, in terms of cumulative firm and social environmental welfare, $SEW_2 + \theta_2$, we observe from the right panel of Figure D.2 that the nucleolus mechanism outperforms both the Shapley and the adjusted TUR mechanism across varying levels of the carbon price, p_t. This is driven by the fact that the nucleolus mechanism offers both greater firm welfare as well as higher incentives for adopting emission abatement technologies. The nucleolus mechanism also performs better than the baseline TUR mechanism at low and moderate levels of the carbon price. This is because the nucleolus avoids double counting and as such delivers a higher level of welfare to firm 2. However, at higher levels of p_t, this is offset by the gains in SEW_2 by the baseline mechanism which offers superior incentives for the adoption of emission abatement technologies.

Appendix E

Chapter 4 – Proofs and Numerical Parameters

Proof of Theorem 4.1: Consider an arbitrary location u in the region $\mathcal{R}$ with N bike-sharing stations distributed uniformly across a region of radius R. We now obtain the average distance to the k^{th} nearest station from u, $\langle r_k(N) \rangle$. Let $P(r)dr$ denote the probability that the k^{th} nearest station is located at a distance between r and $r + dr$ from u. Equivalently, it is the probability that $k-1$ of the other $N-1$ stations lie within a radius of r and at least one of the remaining $N-k$ stations lies inside the ring of radii r and $r+dr$. Therefore,

$$\begin{aligned}
P(r)dr &= \binom{N-1}{k-1} \left(\frac{r^2}{R^2}\right)^{k-1} \left[\sum_{i=1}^{N-k} \binom{N-k}{i} \left(\frac{2rdr}{R^2}\right)^{i}\right] \\
&= \binom{N-1}{k-1} \left(\frac{r^2}{R^2}\right)^{k-1} \left[\binom{N-k}{1} \left(\frac{2rdr}{R^2}\right)\right] \quad \text{(ignoring higher order terms)} \\
&= \frac{2(N-k)}{R} \binom{N-1}{k-1} \left(\frac{r}{R}\right)^{2k-1} dr.
\end{aligned}$$

The average distance to the k^{th} nearest station, $\langle r_k(N) \rangle$, is then given by,

$$\begin{aligned}
\langle r_k(N) \rangle &= \int_{r=0}^{R} rP(r)dr \\
&= \int_{r=0}^{R} 2(N-k) \binom{N-1}{k-1} \left(\frac{r}{R}\right)^{2k} dr
\end{aligned}$$

$$= \frac{2(N-k)}{R^{2k}} \binom{N-1}{k-1} \int\limits_{r=0}^{R} r^{2k} dr$$

$$= \frac{2(N-k)}{R^{2k}} \binom{N-1}{k-1} \int\limits_{r=0}^{R} r^{2k} dr$$

$$= \frac{2R(N-k)}{2k+1} \binom{N-1}{k-1}.$$

In order to compute the average access time $\langle \tau_a^B \rangle$ for an individual using the bike-sharing system, we need to compute the average distance to the nearest available bike, and the average distance from the nearest available dock after returning a bike. The symmetry ensures that the two distances are equal. Therefore, $\langle \tau_a^B \rangle$ is then given by twice the time to walk to the k^{th} nearest station conditioned on all the preceding $k-1$ nearer stations being empty, for each k. Further, the probability p of finding an available bike in some station is given by the service level, $p = \nu$.

$$\begin{aligned}
\langle \tau_a^B \rangle &= 2 \sum_{k=1}^{N-1} p(1-p)^{k-1} \langle r_k(N) \rangle \\
&= 2 \sum_{k=1}^{N-1} \frac{2p(1-p)^{k-1} R(N-k)}{2k+1} \binom{N-1}{k-1} \\
&= 4R \left[\sum_{k=1}^{N-1} \frac{\nu(1-\nu)^{k-1}(N-k)}{2k+1} \binom{N-1}{k-1} \right] \quad (p = \nu) \\
&= 4R\gamma\left(N, \nu\right).
\end{aligned}$$

Using hyper-geometric identities in Mathematica 12.1.0, we also obtained a closed-form expression for $\gamma\left(N,\nu\right)$. However, for our present comparative static purposes, it suffices to derive the dependence of $\langle \tau_a^B \rangle$ on R. The preceding analysis is also of independent interest in diverse applied settings, such as statistical physics, wherein similar computations may be required (Bhattacharya and Chakrabarti 2008). □

Proof of Proposition 4.1: An individual with origin-destination (u, v) prefers a car to public transport if and only if $U^C(p) > U^P(p)$. Thus,

$$\theta(p) - \theta_a \tau_a^C(p) - \theta_w \tau_w^C(p) - \tau_g^C(p) > \theta(p) - \theta_a \tau_a^P(p) - \theta_w \tau_w^P(p) - \tau_g^P(p).$$

By comparing the disutilities of the two modes and substituting the expressions from Remark 4.1, we have,

$$\theta_a \tau_a^P + \theta_w \tau_w^P + \theta_g \left(\frac{d(u,v)}{v_P} \right) + K_P + d(u,v) f_P > \theta_g \left(\frac{d(u,v)}{v_C} \right) + K_c + d(u,v) f_C.$$

Rearranging the terms, and assuming that $\theta_g \left[\frac{1}{v_P} - \frac{1}{v_C} \right] + f_P - f_C > 0$, we obtain that the above inequality is equivalent to,

$$d(u,v) > \frac{K_c - \theta_a \tau_a^P - \theta_w \tau_w^P - K_P}{\theta_g \left[\frac{1}{v_P} - \frac{1}{v_C} \right] + f_P - f_C} = \tilde{d}_{CP}.$$

We note that the condition is satisfied so long as v_C is sufficiently greater than v_P as mentioned previously. □

Proof of Proposition 4.2: An individual with origin-destination (u, v) prefers a car to bike-sharing if and only if $U^C(p) > U^B(p)$. Thus, by comparing the disutilities of the two modes of transport and from Remark 4.1, we have,

$$\theta_a \tau_a^B + \theta_g \left(\frac{d(u,v)}{v_B} \right) + K_B + d(u,v) f_B > \theta_g \left(\frac{d(u,v)}{v_C} \right) + K_c + d(u,v) f_C.$$

From Theorem 4.1,

$$4\theta_a R \gamma (N, \nu) + \theta_g \left(\frac{d(u,v)}{v_B} \right) + K_B + d(u,v) f_B > \theta_g \left(\frac{d(u,v)}{v_C} \right) + K_c + d(u,v) f_C.$$

Rearranging the terms, and assuming that v_C is sufficiently greater than v_B, we obtain that the above inequality is equivalent to,

$$d(u,v) > \frac{K_C - K_B - 4R\theta_a \gamma (N, \nu)}{\theta_g \left[\frac{1}{v_B} - \frac{1}{v_C} \right] + f_B - f_C} = \tilde{d}_{CB}.$$

Further, an individual with origin-destination (u, v) prefers public transit to bike-sharing if and only if $U^P(p) > U^B(p)$. Thus, by comparing the disutilities of the two modes of transport and from Remark 4.1 and Theorem 4.1, we similarly have,

$$4\theta_a R \gamma (N, \nu) + \theta_g \left(\frac{d(u,v)}{v_B} \right) + K_B + d(u,v) f_B > \theta_a \tau_a^P + \theta_w \tau_w^P + \theta_g \left(\frac{d(u,v)}{v_P} \right) + K_P + d(u,v) f_P.$$

Rearranging the terms, and assuming that v_P is sufficiently greater than v_B, we obtain that the above inequality is equivalent to,

$$d(u,v) > \frac{K_P - K_B + \theta_w \tau_w^P + \theta_a[\tau_a^P - 4R\gamma\,(N,\nu)]}{\theta_g\left[\frac{1}{v_B} - \frac{1}{v_P}\right] + f_B - f_P} = \tilde{d}_{PB}.$$

□

Proof of Lemma 4.1: The radius of coverage of bike-sharing is given by R. Let $\tilde{R}$ denote the average distance from any point in the interior of the region to a point in the circumference of the region. Then, clearly, on average, for an origin u in the interior of the region, if the destination v is such that $d(u,v) > \tilde{R}$, then v shall lie outside the region of coverage. We now compute $\tilde{R}$ as a function of R. By radial symmetry, $\tilde{R}$ is the average distance of an arbitrary point on the circumference of the region to all points in the interior of the region.

Consider a coordinate system with its origin lying on the circumference of the region and let a diameter of the circular region correspond to one of the coordinate axes. As noted, the average distance of the origin from all points in the interior of the region corresponds to $\tilde{R}$. Employing polar coordinates, we have,

$$\tilde{R} = \frac{1}{\pi R^2}\int_{-\pi/2}^{+\pi/2}\int_{0}^{2R\cos\theta} r^2\,dr\,d\theta = 32R/9\pi.$$

□

Proof of Proposition 4.3:

i. An individual p with origin-destination (u,v) prefers the bimodal option to bike-sharing if and only if $U^{BP}(p) > U^B(p)$. Thus, by comparing the disutilities of the two modes of transport and from Remarks 4.1 and 4.2, we have,

$$\theta_g\left(\frac{d(u,v)}{v_B}\right) + K_B + d(u,v)f_B > \theta_w\tau_w^P + \left[\frac{d(u,v)}{v_P} + \frac{\tau_a^P v_W}{v_B}\right]\theta_g + \\ K_P + K_B + \tau_a^P v_W f_B + d(u,v)f_P.$$

Rearranging the terms, and assuming, as before, that v_P is sufficiently greater than v_B, we obtain that the above inequality is equivalent to,

$$d(u,v) > \frac{\theta_w\tau_w^P + \tau_a^P v_W\left[\frac{\theta_g}{v_B} + f_B\right] + K_P}{\theta_g\left[\frac{1}{v_B} - \frac{1}{v_P}\right] + f_B - f_P} = \tilde{d}_{MB}.$$

ii. An individual p with origin-destination (u,v) prefers the bimodal option to public transit if and only if $U^{BP}(p) > U^{P}(p)$. Thus, by comparing the disutilities of the two modes of transport and from Remarks 4.1 and 4.2, we have,

$$\theta_a\tau_a^P + \theta_w\tau_w^P + \theta_g\left(\frac{d(u,v)}{v_P}\right) + K_P + d(u,v)f_P > \theta_a\tau_a^B + \theta_w\tau_w^P + \left[\frac{d(u,v)}{v_P} + \frac{\tau_a^P v_W}{v_B}\right]\theta_g + K_P + K_B + \tau_a^P v_W f_B + d(u,v)f_P.$$

Rearranging the terms, we obtain that the above inequality is equivalent to,

$$\theta_a(\tau_a^P - \tau_a^B) > \tau_a^P v_W\left(\frac{\theta_g}{v_B} + f_B\right) + K_B.$$

iii. An individual p with origin-destination (u,v) prefers the bimodal option to a car if and only if $U^{BP}(p) > U^{C}(p)$. Thus, by comparing the disutilities of the two modes of transport and from Remarks 4.1 and 4.2, we have,

$$\theta_g\left(\frac{d(u,v)}{v_C}\right) + K_c + d(u,v)f_C > \theta_a\tau_a^B + \theta_w\tau_w^P + \left[\frac{d(u,v)}{v_P} + \frac{\tau_a^P v_W}{v_B}\right]\theta_g + K_P + K_B + \tau_a^P v_W f_B + d(u,v)f_P.$$

Rearranging the terms, and assuming, as before, that v_C is sufficiently greater than v_P, we obtain that the above inequality is equivalent to,

$$d(u,v) < \frac{K_C - K_B - K_P - \theta_a\tau_a^B - \theta_w\tau_w^P - \tau_a^P v_W\left[\frac{\theta_g}{v_B} + f_B\right]}{\theta_g\left[\frac{1}{v_P} - \frac{1}{v_C}\right] + f_P - f_C} = \tilde{d}_{MC}.$$

□

Proof of Theorem 4.2: First, we observe that each rebalancing stage corresponds to a traveling salesman problem (TSP) route that visits each station in the system exactly once. Asymptotic analysis (Daganzo 2005) of a TSP routing that visits N sites randomly distributed in a region with a size A provides an approximate routing distance of $k_{TSP}\sqrt{AN}$ where k_{TSP} is a scalar constant that is determined by the shape of the geographic region served, as well as the distance metric norm (Ansari et al. 2018), and A is the size of the region. Therefore, it immediately follows that the average distance during each rebalancing stage is $k_{TSP}R\sqrt{\pi N}$.

Further, $f(\nu, k, \lambda)$ denotes the rebalancing frequency, i.e. number of rebalancing stages required per unit time, to maintain a service level of ν. Then, $1/f(\nu, k, \lambda)$ corresponds to the time interval between two successive rebalancing stages. K denotes the average capacity of each station, and let X denote the number of bikes/docks utilized in the time interval between two successive rebalancing stages. To maintain a service level of ν, $Pr(X \leq K) = \nu$. Further, as mentioned, we assume that capacity of bikes and docks at each station is utilized according to a Poisson arrival/departure process at a spatial demand imbalance rate of λ per unit time. Then, it follows that $X \sim Poisson(\lambda/f(\nu, K, \lambda))$. Since the cumulative distribution function for a Poisson-distributed random variable Y, $Pr(Y \leq m)$ with mean μ and integer m, is equal to $Q(m+1, \mu)$, where Q is the regularized gamma function, it follows that that, $Pr(X \leq K) = Q\left(K+1, \lambda/f(\nu, K, \lambda)\right) = \nu$. This completes the proof. $\square$

Numerical parameters for Figure 4.2

In Figure 4.2, we substitute realistic parameter values to generate schematic plots that illustrate Propositions 4.1-4.3. θ_a, θ_w and θ_g refer to the disutility for an individual from the time to access a mode of transport, from waiting for the mode of transport, and from the travel time, respectively. Steimetz (2008) estimates the value of travel time to be \$29.46/hr, and we therefore, set $\theta_g = \$0.49/\text{min}$. Further, based on Dickey (1983), we assume that waiting time is worth twice as much to individuals, and walking time 1.5 times as much. This leads to $\theta_a = \$0.74/\text{min}$ and $\theta_w = \$0.98/\text{min}$.

Based on the estimates of average speeds of cars and public transport options (bus, trains, light rails) across different cities, as in Newman and Kenworthy (1999) and Newman (2009), we set the average speed of cars, $v_C = 42$ km/hr, and average speed of public transit, $v_P = 30$ km/hr. We then assume the speed of a bike-share user, $v_B = 13$ km/hr.

Based on estimates from a fare review of Vancouver's public transportation system (Steer Davies Gleave 2016), we assume the average fare for public transit to be $f_P = \$0.30/\text{km}$[1] and set $K_P = 0$. Winters et al. (2019) analyze data from Vancouver's Mobi bike sharing system and find that the mean number of bike-share trips taken by a surveyed set of members is 10.5 trips per month. Since the 3-month pass costs \$75, we then estimate an average fixed cost for bike-sharing per trip of $K_B = \$2.38/\text{trip}$, and set $f_B = 0$. This is in line with the fare structure for most public bike-sharing systems which operate on a subscription based pricing structure. For a private car, we assume the fixed per-trip cost K_C (which incorporates the averaged cost of ownership and cost of parking and so forth) to be \$12.34 and the marginal fuel cost per km, $f_C = \$0.14/\text{km}$ based on estimates from https://carcosts.caa.ca/.

We assume a headway of 6 minutes between buses/metro resulting in an average waiting time for public transit, $\tau_w^P = 3$ minutes. We assume the time to reach the nearest public transit point to be 4 minutes, thereby resulting in $\tau_a^P = 8$ minutes. These numbers are in line with typical access and wait times for public transport systems across cities. We assume the radius of bike-sharing coverage to be 7.5 km resulting in $\tilde{R} = 8.49$ km. Finally, note that, in our model, the average access time to the nearest bike and dock, τ_a^B, is derived from the density of the bike-sharing station using Theorem 4.1. However, for simplicity, in our numerical computations, we directly assume the access time for bike-sharing, $\tau_a^B = 2$ minutes.

[1] For simplicity, we consider a conversion of 1 USD = 1 CAD.