A Combined and Robust Modal-split/Traffic Assignment Model for Rail and Road Freight Transport

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Abstract

Searching for achieving an ambitious reduction in greenhouse gas emissions, the EU has set as a goal a modal shift in freight transport of 30% by rail for the near future. In this context, it is vital to use modal choice models road versus rail to assess the shippers' acceptance of the actions promoting the use of rail. This paper develops a combined model for jointly evaluating modal split and railway freight flows, addressed to the case when a modal split based on a random utility model is available, and some of its coefficients may present a non-negligible variability. To this end, after the initial deterministic formulation a robust counterpart of the model is developed. The model, formulated as a non-linear integer programming problem, is oriented to a multi-carrier environment and includes constraints to consider the interactions between the different types of flows on the railway network, allowing a good evaluation of the cost types of the carriers and the network capacity. An algorithmic solution based on the outer approximation method is shown to provide accurate solutions in a reasonable computational time for the robust and non-robust versions of the model. Examples centered on a section of the Trans-European Transport Network, the TEN-T Core network corridors, are reported to test the model's applicability. Results show that this model can be a helpful tool for analyzing the possible shippers' response to the different railway carriers' services competing with the road.

Keywords: Transportation; rail freight transportation; non-linear mixed-integer optimization; robust optimization; competing operators.

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1. Introduction

Climate-change reduction policies require transportation to be efficient and low-polluting. However, globalization implies a substantial increase in moving goods throughout Europe and, as a consequence, the congestion on roads is reaching unsustainable levels. The EU White Paper on Transport (European Commission (2011)) fixed ten goals for a competitive and resource-efficient transport system, intending to achieve a 60% Greenhouse Gas emission reduction. One of these goals is that "*Thirty percent of road freight over 300 km should shift to other modes such as rail or waterborne transport by 2030, and more than 50 % by 2050*".

The transport of goods by rail involves the participation of different stakeholders, in particular: railway undertakings (rail freight carriers who provide the service of transporting goods), infrastructure managers (who own the infrastructure and are in charge, among other tasks, of allocating capacity on the infrastructure to railway undertakings and setting the associated costs), national regulatory bodies (in charge of ensuring fair and non-discriminatory access to the rail network to all railway undertakings, as stated by European Court of Auditors (2016)) and national safety authorities. Finally, shippers will choose the method of transportation which best suits their needs. The EU's policy objectives for shifting goods from road to rail have been translated into a series of EU legislative measures aiming to open the market, ensuring non-discriminatory access and promoting interoperability and safety. Consequently, formerly integrated railway companies have been separated into national infrastructure managers and railway undertakings, and the rail freight market was fully open to competition by 1 January 2007.

Rail freight is in direct competition with the road: shippers regularly compare both when deciding which mode of transport to use, taking mainly into account: price, frequency, transport time, reliability, and quality of service to the customer. Recently, the impact that transport mode has on greenhouse gas emissions is also crucial for making a choice.

In recent years, several public sector national, international, and regional freight transport models have been developed and improved to increase the understanding of the impacts of transport policies on shippers, forwarders, carriers, and the environment (de Jong et al. (2013)). These models rely on different methodologies and approaches in the scientific literature that deal with the complexity and needs of freight transportation models (Meersman et al. (2016)), such as including various modes of transportation and the variability and seasonality of supply and demand of goods.

This paper develops a combined modal-split/traffic assignment model for evaluating the train-road modal share in future scenarios, or also to the case when a modal split model based on random utilities is available, and some of its coefficients may present a non-negligible range of variability. The assignment of railway flows considers its various components in a multi-carrier environment, including explicit constraints when interactions occur between the different types of flows on the railway network, allowing a good evaluation of the various cost types of the carriers and the network capacity. A robust counterpart of the model, based on the robustness concept developed in Koster et al. (2013), is formulated in order to take into account more conservative modal splits under a limited worst-case standpoint. An algorithm based on the outer approximation of Duran & Grossmann (1986) is developed to solve the resulting non-linear integer problems in a reasonable computational time.

The remainder of this article is organized as follows. Section 2 summarizes the most relevant state-of-the-art approaches to the topics covered in the paper. The model is developed in Section 3 as a mixed integer non-linear programming model and in section 4 its robust counterpart is developed in order to deal with the uncertainty in the coefficients of the disutilities. Section 5 details the algorithm proposed to solve the optimization problem. Section 6 describes a case study to show the applicability and computational viability of the model. Finally, Section 7 summarizes the main conclusions.

2. Literature Review

For a long time, rail freight transport has not been studied as intensively as rail passenger transport. At the strategic level, the earlier multimode-multiproduct traffic assignment models by Guelat et al. (1990) and Crainic et al. (1990) state normative models for the distribution of freight flows through various interacting modes. The model presented in Fernández L. et al. (2004) is oriented to the analysis of freight rail networks' performance. It is formulated as a variational inequality and considers a prioritizing treatment for commodities and the distribution of empty rail cars, jointly with the assignment over the rail network of products to be transported. A very detailed representation of rail freight operations at yards is included. More recently, in the optimization model developed in Maia & do Couto (2014), the authors present a support tool based on a strategic traffic assignment model designed to model macro networks with a high aggregation level, being exclusively designed for freight traffic. The model contemplates road and rail transport modes and considers two types of commodities: intermodal cargo, usually transported in containers, and general cargo, which does not accept intermodality. The goal is to analyze the impact that new links or the improvement of some existing links have on rail freight share. Following the same purpose, the model presented in Rosell & Codina (2020) considers relatively low costly actions on the network for improving capacity by adding new blocking/control systems at a specific location. Also, it analyzes the impact that these actions have jointly on rail operation and infrastructure management.

The application of freight planning models in evaluating policies and actions taken by authorities and governments is abundant in the academic literature. The work in Crisalli et al. (2013) presents a methodology to evaluate rail-road policies such as new services or incentives for long-distance freight transport. They test different examples based on the purposes of the Italian National Plan in long-distance freight transport. Also, in Abate et al. (2018), authors present a disaggregated stochastic model of transport chain and shipment size choice, which is compared with the existing Swedish national model, based on disaggregated data but deterministic. The detailed analysis about freight transport chains presented in Jensen et al. (2019) also highlights the importance that freight transport models have for the EU.

A good perspective about freight transportation models commercially available is offered in Friesz & Kwon (2007). They analyze five key commercial models and how they deal relative to a list of criteria that an ideal freight planning model should correctly address. The authors recommend more research efforts to some essential aspects, such as the simultaneous treatment of shippers and carriers, the necessity of integrating computable general equilibrium models with network models, the inclusion of backhauling and fleet constraints, considering an imperfect competition, including validation of data in the process, and taking into account the revenue management.

International freight transport demand models need to include freight flows between countries as well as internal flows in the countries, involving data from different sources, most of them not available for third parties.

As a consequence, one of the big challenges for building freight transportation models is the quality of data (Meersman et al. (2016), Friesz & Kwon (2007), de Jong et al. (2016)). In Arencibia et al. (2015) discrete choice models are applied to analyze the main factors that determine modal choice in freight transportation, focusing on Spain and Europe's flows. They use a stated preference survey where the population being studied is limited to the shipper (or receiver) companies. Transport cost, travel time, frequency, and delays are factors determining the utility of the alternatives. Another way for estimating the utility parameters on a modal choice model is by using observed data, either from public or private databases (Crisalli et al. (2013), Hwang & Ouyang (2014)) or from official statistics (Zhang et al. (2015)), which usually provide aggregate data.

As far as we know, the freight planning models use separate modal split and assignment. In urban passenger's transport, combined modal-split/traffic assignment models have been developed long ago (Dafermos (1976), Florian (1977), Florian & Nguyen (1978), Abdulaal & Leblanc (1979)). These combined modes have been continuously adapted to different scenarios in the urban passenger transportation context. Thus, recently a combined modal split and assignment model with deterministic travel demand is proposed in Li et al. (2009) for intercity bus and train modes for economically related cities. Also, in Hou et al. (2020) a combined modal split/traffic assignment is developed, taking into account park-and-ride facilities. In the case of freight transportation, the validation of models is done using separate steps, as in Jourquin (2016), where they develop a methodology adapted to the case of limited and heterogeneous sources of information, specially suited for the Trans-European Network projects. However, up to our knowledge, no similar models have been adapted or extended to the case of freight transportation. Our model may help to have a joint view of the more probable shippers' modal choice criteria while highlighting the most attractive rail paths for freight transport. Thus, our model may be part of a decision-making tool for designing and improving the carriers' offer of services.

Objective of the work and contributions. A combined modal-split/traffic assignment model is developed for rail versus road freight transport in multi-operator scenarios. The aim is to obtain consistent train-road modal splits when a modal split model based on random utilities is available to assess changes in the railway system, but its predictive capabilities can be affected because of reasons like:

- limited quality of the input data. They may come from heterogeneous sources or aggregate values, e.g., from official statistics or databases supplemented with aggregated data. As a result, all or part of the model's coefficients may present considerable uncertainty, this being contributed by the extremely low use of train in some countries;

- it has been obtained through stated preference surveys where possible capacity limitations are not reflected, and it cannot be established a priori where they will take place. However, it may subsequently occur due to technical deficiencies in implementing future actions on the railway network.

The predictive role to which the model is addressed can be contrasted taking into account its robust version where it is allowed that a limited number of elements of the utilities can deviate from their nominal values simultaneously. The model does not strictly impose operator's competition, but it does exclude those who do not obtain benefits. Railway carriers' offer of services depends on its profitability, limited by the infrastructure's characteristics and rolling stock availability. Also, our model includes a set of constraints to consider the interactions between the different types of flows on the railway network (flows of product types, flows of railcars, either empty or full, flows of formed trains) and their characteristics.

3. Model description

The railway network will be modeled using an undirected graph $\bar{G} = (N, E)$, in which edges $e \in E$ in the graph have a direct correspondence with tracks, and yards, terminals and diverting/crossing points will be represented by nodes $i \in N$. Because of the bi-directionality of rails, this will be equivalent to working with a directed graph $G = (N, A)$ where, for each edge $e \in E$ two links $a = (i, j)$ and its opposite $-a = (j, i)$ will exist in A. Each arc is assumed to have homogeneous physical characteristics along its length, i.e., we can assume trains run on each of them at constant speed.

Products will move through the network from origin points to destination points and we will specifically refer to them as *terminals*. The demand for products for the time horizon studied is assumed to be known in advance and will be associated to the set of possible origin-destination terminal pairs (OD-pairs) on the network. When describing multicommodity flows a multiple superscript $\omega = (\mathfrak{o}(\omega), \mathfrak{d}(\omega), \mathfrak{p}(\omega))$ will be used, where $\mathfrak{o}(\omega)$, $\mathfrak{d}(\omega)$ and $\mathfrak{p}(\omega)$

are the origin $\mathfrak{o}$, destination $\mathfrak{d}$ and product type $\mathfrak{p}$ respectively in triple ω. By W it will be designated the set of all these triples.

The amount of demand of products of type $\mathfrak{p}(\omega)$ to be transported from origin $\mathfrak{o}(\omega)$ to destination $\mathfrak{d}(\omega)$ during a given period $\mathcal{T}$ (for instance, yearly) will be denoted by χ^ω. For a given OD-pair, the set of paths on the network joining the origin terminal $\mathfrak{o}(\omega)$ with the destination terminal $\mathfrak{d}(\omega)$ will be denoted by $R(\omega)$ and the set containing all the paths will be $R = \cup_{\omega \in W} R(\omega)$. Paths between origin terminals and destination terminals will be referred to as t-paths. Each t-path will be operated by one carrier o within the set $\mathcal{O}$ of railway undertakings or carriers. Each OD-pair will be assumed to be joined by at least one t-path.

Let h_r^ω be the total demand during period $\mathcal{T}$, or flow, transported by train for OD-pair and product ω using t-path r, and let $h^\omega = \sum_{r\in R(\omega)} h_r^\omega$ and $\tilde{h}^\omega$ be the total demand transported by train and by truck, respectively, for OD-pair and product. Variables h_r^ω and $\tilde{h}^\omega$ can be grouped in flow vectors $\mathbf{h}^\omega = (..., h_r^\omega, ...)^\top \in \mathbb{R}^{|R(\omega)|}$, $\omega \in W$, $\mathbf{h} = (..., \mathbf{h}^\omega, ...)^\top \in \mathbb{R}^{|W|}$ and $\tilde{\mathbf{h}} = (..., \tilde{h}^\omega, ...)^\top \in \mathbb{R}^{|W|}$, for convenience (here $\top$ denotes transpose). Let $\tilde{u}^\omega, u_r^\omega$ be the generalized cost or disutility, for OD-pair and unit of product type ω, when transported by truck and by train using t-path $r \in R(\omega)$, respectively.

For an initial description of the model, the remaining variables (flow of railcars, locomotives, flow of trains between yards) will be detailed later in next subsection 3.2 and will be assumed to be comprised in a generic vector of variables $\mathbf{y}$ lying in a specific domain $\mathcal{Y}$. Variables $\mathbf{h}, \tilde{\mathbf{h}}$ and $\mathbf{y}$ will be related each other by some binding constraints $g_\ell(\mathbf{h}, \mathbf{y}) \leq 0, \quad \ell = 1, ..., m$. The model is formulated as the following non-linear optimization problem:

$$\min_{\mathbf{h},\tilde{\mathbf{h}},\mathbf{y}} \quad F(\mathbf{h}, \tilde{\mathbf{h}}) = \sum_{\omega \in W} \left[\sum_{r \in R(\omega)} u_r^\omega h_r^\omega + \int_0^{\tilde{h}^\omega} G_\omega^{-1}(s) ds \right] \tag{1}$$

$$\text{s.t.} \quad \sum_{r \in R(\omega)} h_r^\omega + \tilde{h}^\omega = \chi^\omega \qquad \omega \in W \tag{1a}$$

$$g_\ell(\mathbf{h}, \mathbf{y}) \leq 0 \qquad \ell = 1, .., m \tag{1b}$$

$$\mathbf{y} \in \mathcal{Y} \tag{1c}$$

$$h_r^\omega \geq 0 \qquad r \in R(\omega),\ \omega \in W \tag{1d}$$

$$\tilde{h}^\omega \geq 0 \qquad \omega \in W \tag{1e}$$

As expressed in (1a) the total freight demand (χ^ω) has to be equal to the sum of the demand on the railway system (first term) plus the demand on the truck system (second term). In the objective function (1), $G_\omega^{-1}(\cdot)$ is the inverse demand function $G_\omega^{-1}(\tilde{h}^\omega) = \tilde{u}^\omega + \log\left(\frac{\tilde{h}^\omega}{\chi^\omega - \tilde{h}^\omega}\right)$ (see Sheffi (1985), chapter 6). After some calculation, the objective function in (1) can be stated as:

$$F(\mathbf{h}, \tilde{\mathbf{h}}) = \sum_{\omega \in W} \left[(\chi^\omega - \tilde{h}^\omega) \log \frac{\chi^\omega - \tilde{h}^\omega}{e^{-u^\omega}} + \tilde{h}^\omega \log \frac{\tilde{h}^\omega}{e^{-\tilde{u}^\omega}} - \chi^\omega \log \chi^\omega \right] \quad (2)$$

where the terms $\exp(-u^\omega)$ and $\exp(-\tilde{u}^\omega)$ can be interpreted as proportional to a priori probabilities of choosing rail and truck respectively, and $u^\omega \triangleq (\sum_{r \in R(\omega)} u_r^\omega h_r^\omega)/(\sum_{r \in R(\omega)} h_r^\omega)$ is the mean generalized cost for the train mode $\omega \in W$. Thus, the objective function can be interpreted as a -minus-relative entropy and the model pursues to find the closest modal share to the disutilities $u_r^\omega, \tilde{u}^\omega$ available from the random utility model (RUM).

Let ϑ^ω, ξ_r^ω and η^ω be the Lagrange multipliers of constraints (1a), (1d) and (1e), respectively. Also, γ_r^ω result from the Lagrange multipliers ζ_ℓ of constraints (1b) as $\gamma_r^\omega = \sum_{g_\ell(\mathbf{h},\mathbf{y})=0} \zeta_\ell \frac{\partial g_\ell}{\partial h_r^\omega}$. From the first order conditions of problem (1), and taking into account that Lagrange multipliers η^ω must be finite, the following expression can be derived:

$$\vartheta^\omega = \min_{r \in R(\omega)} \{u_r^\omega + \gamma_r^\omega\}, \quad \omega \in W \quad (3)$$

and also results the modal split following a logit model:

$$\frac{\tilde{h}^\omega}{\chi^\omega} = \{1 + \exp(\tilde{u}^\omega - \vartheta^\omega)\}^{-1} \quad (4)$$

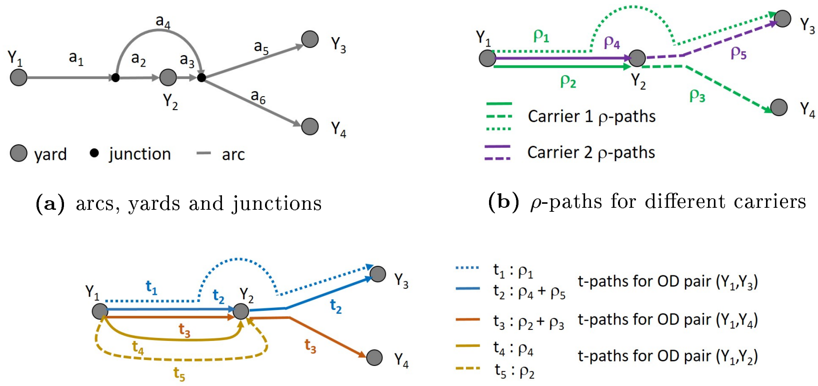
See Appendix B for details about the modal choice properties of the model.

It must be noted that in the previous logit-like expression (4) for the fraction of products shipped by road, the utilities of the rail alternative appear now to be ϑ^ω, i.e., the initially stated utilities u_r^ω are modified by multipliers γ_r^ω corresponding to constraints (1b), having an effect of explicit or implicit capacities. In the next section it will be shown the functional form of the constraints (1b) which will turn out to be linear. Including side capacity constraints in equilibrium models can also be found in Larsson & Patriksson (1994), where the corresponding Lagrange multipliers are interpreted as additional delays or costs. We also interpret here the inclusion of the side constraints (1b) when evaluating the modal share as a correction for the previously evaluated utilities u_r^ω that may come from a RUM model in which these constraints associated to flows could not be taken properly into account when estimating the RUM model.

3.1. Elements of the model

At some points in the network, railcars may be re-classified to assemble outgoing trains from incoming ones. These points will be referred to specifically in this paper as *yards*. In addition, it is assumed that suitable facilities exist for unloading incoming railcars and for reloading other railcars capable of using the outgoing tracks. The compatibility of track gauges determines the configuration of these facilities. Terminals are considered a particular type of yard in which a net amount of products enters or leaves from the "external world" and thus, new trains must be formed or, on the contrary, railcars are left empty and available to form new trains. Terminals usually consist of an intermodal connection point. The set of yards will be denoted by Y, while the set of terminals by $T \subseteq Y$. Finally, diverting/crossing points consist of points at which several tracks may merge, where two opposite trains can cross, or where overtaking between trains may occur.

Given that rail freight transport is, in general, a deregulated competitive market in most countries, it is necessary to consider the effect of several carriers competing under possibly some regulated conditions. Each carrier $o \in \mathcal{O}$ operates a set of corridors, which are composed of lines. Each line can be run in both senses and can be decomposed into two directed lines. Each directed line will be referred to as ρ-path and denoted by symbol ρ, and has one yard as the origin and another different yard as the destination. Each ρ-path is composed of a subset of arcs from set A that continuously connect both two yards. Because it is possible to have different ways to connect two different yards, it is necessary to previously define exactly the subset of arcs that composes each ρ-path. The set of ρ-path for each carrier will be denoted by $\Gamma(o)$, and $\Gamma = \cup\Gamma(o)$ is the disjoint union of all carrier ρ-paths. Also, let $Y(o) \subseteq Y$ be the subset of yards which are origin or destination of at least one ρ-path operated by carrier $o \in \mathcal{O}$. Given an arc $a \in A$, and a carrier $o \in \mathcal{O}$, let $\Gamma(a, o)$ be the subset of $\rho \in \Gamma(o)$ containing the arc a. Figure 1a illustrates with an example the basic elements of the network: arcs, yards



(a) arcs, yards and junctions

(b) ρ-paths for different carriers

(c) t-paths for connecting OD-pairs

Fig. 1. Railway Network elements representation

and junctions. Besides, Figure 1b depicts two carriers and their ρ-paths.

Let $R(o)$ be the set of t-paths between terminals offered by carrier o. Given a t-path $r \in R(o)$, it can be considered as composed by a subset of ρ-paths owned by the carrier o, $\rho \in \Gamma(o)$, that connect the t-path origin terminal to the t-path destination terminal in a continuous way (having different stops, defined by yards that are part of each ρ-path). Figure 1c shows different t-paths connecting Y_1, Y_2, Y_3 and Y_4 terminals. Note that both t_1 and t_2 connect Y_1 and Y_3, but t_2 has one stop at yard Y_2.

Also, $R(\rho)$ will denote the set of t-paths containing ρ as part of their composition. ρ-paths between yards are assumed to have homogeneous characteristics accordingly to the types of rolling stock allowed on them, mainly differences in track gauges or loading gauges. Then, the set of gauges on a ρ-path is assumed to be homogeneous on the track segments composing the ρ-path. This characteristic does not necessarily apply to t-paths between terminals. Given a yard $i \in Y$, Γ_i^+, Γ_i^- will denote the subset of ρ-paths outgoing or incoming into i, respectively, and $\Gamma_i^+(o)$, $\Gamma_i^-(o)$ the same, but limited to the ρ-paths owned by the carrier o .

Let $\mathcal{V}$ be the set of railcar types. It will be assumed that each type of product can be transported by only a subset of railcar types. For a given ρ-path, $\mathcal{V}(\rho)$ will denote the set of railcar types $v \in \mathcal{V}$ that can run on ρ. Also, railcars within a railcar type may circulate on more than one gauge. $\Gamma(v, o)$ represents the subset of ρ-paths compatible with v-type railcar and operated by carrier $o \in \mathcal{O}$, while $\Gamma_i^+(v, o)$, $\Gamma_i^-(v, o) \subseteq \Gamma(v, o)$ represent the same, but restricted to ρ-paths emergent from $i \in Y$ or incident to

$i \in Y$, respectively. Rail freight transport uses different types of locomotives, with different characteristics, as maximum speed, maximum weight, or weight/speed ratio. Also, as in the case of railcars, not all locomotives are compatible with all types of tracks. Let K_M be the set of freight locomotive types, and $K_M(\rho) \subseteq K_M$, the subset of $k \in K_M$ compatibles with ρ.

Finally, the road network, the alternative transport mode, is represented by additional links that directly connect each OD-pair's origin and destination. Table A.3 in Appendix A summarizes the list of sets.

3.2. Relationships for carriers' rail transport flows

Shippers need their products to be transported from origin to destination, having two options. On the one hand, rail carriers provide rail freight transportation services, and on the other, different carriers offer road freight transportation services. This subsection details rail carriers' transport conditions to link rail demand with the way products are transported by train.

In rail transportation, products are transported in railcars. Units of freight to be transported by train will be limited by the railcars' maximum load. Let $\alpha^{v,\mathfrak{p}(\omega)}$ be the parameter for the maximum load per unit of product $\mathfrak{p}(\omega)$ on railcar of type v, and $f_\rho^{v,\omega}$ the variable which represents the loaded railcars with product $\mathfrak{p}(\omega)$ of type v that run on ρ and go from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$. Equation (5) states for products of type $\mathfrak{p}(\omega)$ transported by rail from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ moved on a given directed line ρ operated by carrier $o \in \mathcal{O}$. The left hand of the inequality is for the amount of freight, which should be less or equal to the sum of the maximum loading capacity available on all v-type railcars compatibles with ρ.

$$\sum_{r \in R(\rho)} h_r^\omega \leq \sum_{v \in \mathcal{V}(\rho)} \alpha^{v,\mathfrak{p}(\omega)} f_\rho^{v,\omega} \qquad \forall \omega \in W,\ \forall \rho \in \Gamma(o),\ \forall o \in \mathcal{O} \qquad (5)$$

Carrier conditions for transporting products are mainly related to the physical characteristics of rail transportation: track features, trains' length and weight, and capacity limits on tracks and yards. Transportation services provided by carriers also influence shippers' choices. The following equations gather rail freight transportation characteristics and conditions with carrier flow requirements. First, equation (6) below defines the total flow, F_ρ^v, of railcars of type v that run on line ρ. Here, variables $f_\rho^{v,\emptyset}$ represent empty railcars. Clearly, railcars of type v should not run on line ρ if they are not compatible. Ideally, the aim is that railcars should run along the entire network, and yards have no spare units of railcars. At each yard and for each carrier, the entrance flow of v-type railcars belonging to carrier o must be equal to the exit flow of that railcars. Also, diverting/crossing points have to be balanced on entries and exits. Then, equation (7) sets a balance on nodes, for each type of railcar and each carrier.

$$F_\rho^v = \begin{cases} f_\rho^{v,\emptyset} + \sum_{\omega \in W} f_\rho^{v,\omega} & \forall v \in \mathcal{V},\ \forall \rho \in \Gamma(v,o),\ \forall o \in \mathcal{O} \\ 0 & v \text{ and } \rho \text{ incompatibles} \end{cases} \tag{6}$$

$$\sum_{\rho \in \Gamma_i^-(v,o)} F_\rho^v = \sum_{\rho \in \Gamma_i^+(v,o)} F_\rho^v \quad \forall i \in N,\ \forall v \in \mathcal{V},\ \forall o \in \mathcal{O} \tag{7}$$

Let m_ρ^k be the flow of trains of type k on line ρ. The maximum length for a train that runs on a directed line ρ will be conditioned mainly by the maximum train length allowed on track sidings for the tracks that are part of the line and for the maximum length for shunting movements on yards that are the origin or destination of the line. Let ℓ^v be the length of v-type railcars, and let $\bar{\ell}_\rho$ be the maximum train length allowed on ρ. Equation (8) states limitation for flows based on average length: the sum of lengths of all railcars that run on a line ρ should be less or equal than the sum of all trains that run on the line multiplied by the maximum length allowed on the line.

$$\sum_{v \in \mathcal{V}(\rho)} \ell^v F_\rho^v \leq \bar{\ell}_\rho \sum_{k \in K_M} m_\rho^k \qquad \forall \rho \in \Gamma(o),\ \forall o \in \mathcal{O} \tag{8}$$

Also, there are limits on maximum train tonnage. In this case, the locomotive characteristics (relationship between speed and load), track features (slopes) or normative (axle load limits) condition maximum train weight. Let α^v be the tare of v-type railcars, $\alpha^{v,\mathfrak{p}(\omega)}$ the average weight for product $\mathfrak{p}(\omega)$ transported on v-type railcars and $\bar{\alpha}_\rho^k$ the maximum weight allowed for k-type locomotives running on line ρ. As before, Equation (9) states a limitation for flows based on average tonnage: the sum of the weight of all railcars that run on line ρ should be less or equal than the sum of all trains that run on the line multiplied by the maximum train tonnage allowed on the line.

$$\sum_{v \in \mathcal{V}(\rho)} (\alpha^v F_\rho^v + \sum_{\omega} \alpha^{v,\mathfrak{p}(\omega)} f_\rho^{v,\omega}) \leq \sum_{k \in K_M} \bar{\alpha}_\rho^k m_\rho^k \quad \forall \rho \in \Gamma(o),\ \forall o \in O \tag{9}$$

Infrastructure managers are in charge of allocating capacity on the infrastructure for carriers disposal, and carriers, in consequence, buy the slots that interest them among those that are available. These slots limit the maximum number of trains a carrier can operate in each directed line. N_ρ represents carriers capacity allocation on ρ-path and imposes a limit on the maximum number of trains on that directed line, as stated by constraint (10). Likewise, the tracks capacity limit, N_a, restricts the maximum number of trains that run on track a; this is represented by (11).

$$\sum_{k \in K_M} m_\rho^k \leq N_\rho \qquad \forall \rho \in \Gamma(o), \forall o \in \mathcal{O} \tag{10}$$

$$\sum_{o \in \mathcal{O}} \sum_{\rho \in \Gamma(a,o)} \sum_{k \in K_M} m_\rho^k \leq N_a \qquad \forall a \in A \tag{11}$$

A railcar may be part of different convoys during the trip if the t-path has some intermediate yards distinct from the origin and the destination. Each additional stop and composition or decomposition of trains increases the total travel time and the total costs. So, it is important to know where trains are mounted and dismounted. Let us define the variable $\theta_{i',i}^{k,o}$ as the number of trains of type k operated by carrier o that are mounted at yard $i' \in Y(o)$ and dismounted at yard $i \in Y(o)$, $i' \neq i$. Also, let $m_{\rho,i}^k$ be the variable for the number of trains of type k that run on each line ρ operated by carrier o, with destination yard i. The total number of trains of type k running on line ρ, m_ρ^k, verifies (12), while the relationship between $m_{\rho,i}^k$ and $\theta_{i',i}^{k,o}$ will be given by the balance equations (13):

$$m_\rho^k = \sum_{i \in Y(o)} m_{\rho,i}^k \qquad \forall k \in K_M,\ \forall \rho \in \Gamma(o),\ \forall o \in \mathcal{O} \tag{12}$$

$$\sum_{\rho \in \Gamma_{i'}^{+}(o)} m_{\rho,i}^k - \sum_{\rho \in \Gamma_{i'}^{-}(o)} m_{\rho,i}^k = \theta_{i',i}^{k,o} \quad \forall k \in K_M,\ \forall i', i \in Y(o), i' \neq i,\ \forall o \in \mathcal{O} \tag{13}$$

Next constraints (14) limit the total incoming and outgoing flow of trains that can be dismounted and mounted, respectively on a yard $i \in Y$, accordingly to the yard's capacity in number of trains (parameter $\tilde{N}_i$).

$$\sum_{o\in\mathcal{O}}\sum_{i'\in Y(o)}\sum_{k\in K_M}\theta_{i,i'}^{k,o}\leq\tilde{N}_i,\qquad\sum_{o\in\mathcal{O}}\sum_{i'\in Y(o)}\sum_{k\in K_M}\theta_{i',i}^{k,o}\leq\tilde{N}_i\quad\forall i\in Y\tag{14}$$

Rolling stock is expensive. Carriers try to adjust the number of railcars and locomotives to their service needs. An estimation based on Little's law (see, e.g. Little (1961)) is applied to state lower bounds for the number of railcars and locomotives a carrier needs to provide the service. Then, let $\bar{\mathcal{T}}$ be a parameter for the effective time that rolling stock runs during the period $\mathcal{T}$. For instance, if $\mathcal{T}$ corresponds to one year expressed in hours , $\bar{\mathcal{T}}$ is the number of effective hours available. This estimation using Little's law may be appropriate especially when the requested shipments to the carriers follow regular patterns. The effect of irregular demand patterns may be taken into account by decreasing parameter $\bar{\mathcal{T}}$ applying the peak factors of the demand patterns. Parameter t_ρ is the average run time for one train in line ρ, taking into account necessary layovers: t_ρ could be calculated from the average travel time weighted by type of locomotive, plus an extra time for the waiting time related to the arrival to destination yard, or the exit from the origin yard. Variable $\lambda^{v,o}$ represents the minimum number of v-type railcars the carrier o needs to provide the service. Following Little's law, the first inequality on the equation (15) states that the average number of railcars needed to perform the service is equal to the sum of the number of railcars that run on a line multiplied by the average time spent on that line. The second inequality is a bound on the number of railcars of type v available for operator o, which is specified by parameter $L^{v,o}$. Equation (16) is the equivalent of (15) for locomotives, being the parameter $\hat{L}^{k,o}$ the maximum number of k-type locomotives the carrier o may need.

$$\frac{1}{\bar{\mathcal{T}}}\sum_{\rho\in\Gamma(o)}t_\rho F_\rho^v\leq\lambda^{v,o}\leq L^{v,o}\qquad\forall v\in\mathcal{V},\ \forall o\in\mathcal{O}\tag{15}$$

$$\frac{1}{\bar{\mathcal{T}}}\sum_{\rho\in\Gamma(o)}t_\rho m_\rho^k\leq\hat{L}^{k,o}\qquad\forall k\in K_M,\ \forall o\in\mathcal{O}\tag{16}$$

3.3. Carrier-Shipper relationship

Finally, it is essential to consider the cost-effectiveness of carriers. Equation (17) below states that a carrier has no losses, or on the contrary, it is left out and carries out no transportation of goods. The left hand side of inequality (17) represents the total import paid by shippers to a carrier, while the right hand side of the inequality corresponds to direct costs associated with rail transport. The first term is train composition and decomposition costs. The second is the running time cost, while the third term is for renting/maintenance costs of railcars. A *big-M* component is added to this equation with a new binary variable $\hat{y}_0$ also included into an additional constraint (18). Due to the modal choice characteristics of the model none of the modes has the possibility of capturing entirely the demand of a product per O-D pair. Then, a constraint that forces the viability of carriers transportation may cause infeasibility on the model (for instance, when an OD pair is served by only one carrier and this carrier cannot reach enough demand to be competitive). M_o is a constant greater than the maximum carrier cost, and $\bar{\chi}^\omega$ is a small fraction of the total demand χ^ω.

$$\sum_{\omega \in W} \sum_{r \in R(\omega,o)} U_r^\omega h_r^\omega \geq \sum_{k \in K_M} \sum_{i \in Y(o)} \sum_{\substack{j \in Y(o) \\ j \neq i}} (C_{i'}^{k,o} + \tilde{C}_i^{k,o}) \theta_{i',i}^{k,o} + \sum_{k \in K_M} \sum_{\rho \in \Gamma(o)} \hat{C}_\rho^k m_\rho^k + \sum_{v \in \mathcal{V}} D^{v,o} \lambda^{v,o} - M_o(1 - \hat{y}_o) \qquad \forall o \in \mathcal{O} \tag{17}$$

$$\sum_{r \in R(\omega,o)} h_r^\omega \leq \bar{\chi}^\omega + \chi^\omega \cdot \hat{y}_o \qquad \forall o \in \mathcal{O},\ \forall \omega \in W \tag{18}$$

The rest of the parameters are: U_r^ω is the price per unit for transporting $\mathfrak{p}(\omega)$ from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ using carrier path r; $C_{i'}^{k,o}, \tilde{C}_i^{k,o}$ are the cost for train formation at yard i' and train decomposition at yard i, respectively, for k-type train and carrier o; $\hat{C}_\rho^k$ is the cost of a k-type train running on ρ. $D^{v,o}$ is the cost for renting/maintenance of v-type railcars, for carrier o. Obviously, these are not the unique costs associated with rail transport. So, to avoid the lack of information for other costs, it is advisable to apply a percentage of increment on these costs when the model is applied. Appendix C shows a summary of the different components of the costs used for the test.

Finally, to complete the model, the domain of variables is as follows:

$$h_r^\omega, \tilde{h}^\omega \in \mathbb{R}^+ \tag{19}$$

$$f_\rho^{v,\omega}, f_\rho^{v,\emptyset}, m_{\rho,j}^k, \lambda^{v,o}, \theta_{i',i}^{k,o} \in \mathbb{Z}^+,\ \hat{y}_o \in \{0,1\} \tag{20}$$

Table A.4 shows the list of parameters the model requires, while Table A.5 summarizes the list of variables used in the model (see Appendix A).

3.4. Deterministic version of the optimization problem

In previous subsections, we have detailed the elements of the model related to flows of trains and railcars with flows of products on the network defining new variables and constraints. Particularly, the vector of variables $\mathbf{y}$ in problem (1) comprises: $\mathbf{y} \equiv f_\rho^{v,\omega}, f_\rho^{v,\emptyset}, m_\rho^k, \lambda^{v,o}, \theta_{i',i}^{k,o} \in \mathbb{Z}^+, \hat{y}_o \in \{0,1\}$, while the vector of variables $\mathbf{x}$ comprises $\mathbf{x} \equiv h_r^\omega, \tilde{h}^\omega$. Then, problem (1) can be stated as the following mixed integer non-linear problem **MINLP-D**:

(MINLP-D) (21)

$$\min_{h,\tilde{h},f,m,\lambda,\theta,y_o} \quad \sum_{\omega\in W}\sum_{r\in R(\omega)} u_r^\omega h_r^\omega + \sum_{\omega\in W} \tilde{u}^\omega \tilde{h}^\omega + \sum_{\omega\in W} \int_0^{\tilde{h}^\omega} \left(\log \frac{x}{\chi^\omega - x}\right) dx$$

$$\text{s.t.} \quad (1a), (1d), (1e), (5) - (20),$$

where the "-D" is an acronym for "deterministic". In the next section, the robust counterpart of problem **MINLP-D** is developed taking into account the uncertainty in the parameters u_r^ω, $\tilde{u}^\omega$

4. Robustness on Utility Function

In this section the uncertainty in the generalized costs, or disutilities, u_r^ω, $\tilde{u}^\omega$ for transporting products $\mathfrak{p}(\omega)$ from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ is dealt with, developing a model under the scope of robust optimization. We assume that the systematic component of the disutilities for the rail and road transport modes are given by affine functional forms of m and $\tilde{m}$ explanatory variables as in (22). Typically these explanatory variables are travel time, price, distance, GHG (Greenhouse Gas) emissions, among others.

$$u_r^\omega = \beta_0^\omega + \sum_{j=1}^{m} \beta_j^\omega u_{r,j}^\omega, \qquad \tilde{u}^\omega = \tilde{\beta}_0^\omega + \sum_{j=1}^{\tilde{m}} \tilde{\beta}_j^\omega \tilde{u}_j^\omega \tag{22}$$

A critical step is to obtain a good estimation of the parameters β and $\tilde{\beta}$ by using glm regression, for instance. It is not too hard to obtain reasonable estimates for the utility function parameters' mean value and confidence intervals. From them, the uncertainty of parameters β may be expressed as follows:

$$\beta_j^\omega \in [\beta_j^{-,\omega} - \beta_j^{+,\omega}, \beta_j^{-,\omega} + \beta_j^{+,\omega}],\ j = 0, \ldots, m, \quad \forall \omega \in W \tag{23}$$

$$\tilde{\beta}_j^\omega \in [\tilde{\beta}_j^{-,\omega} - \tilde{\beta}_j^{+,\omega}, \tilde{\beta}_j^{-,\omega} + \tilde{\beta}_j^{+,\omega}],\ j = 0, \ldots, \tilde{m}, \quad \forall \omega \in W \tag{24}$$

Our approach is based on the robustness concept developed in the work by Koster et al. (2013). Following this work, the number of parameters that may take its worse value is restricted to a (small) value H, and in this way, it is possible to set the level of conservatism and robustness of the solutions (The greater the value for H, the greater the uncertainty on parameters and the robustness of the model solutions). Details about how robustness is applied in the utility function are shown in Appendix D. We can reformulate the problem by replacing each element $u_r^\omega \cdot h_r^\omega$ in the objective function by a new expression as it appears in (25), and adding the new set of constraints (26), where π, p are auxiliary variables required for the reformulation:

$$\min_{h,\pi,p\geq 0} \quad \sum_{\omega} \sum_{r\in R(\omega)} [\ (\beta_{r,0}^{-,\omega} + \sum_{j=1}^{m} \beta_{r,j}^{-,\omega} u_{r,j}^\omega) h_r^\omega + H\pi_r^\omega + \sum_{j=0}^{m} p_{r,j}^\omega\ ] \tag{25}$$

$$\pi_r^\omega + p_{r,j}^\omega \geq \beta_{r,j}^{+,\omega} u_{r,j}^\omega h_r^\omega, \quad \pi_r^\omega + p_{r,0}^\omega \geq \beta_{r,0}^{+,\omega} h_r^\omega, \quad \forall j,\ \forall \omega,\ \forall r \in R(\omega) \tag{26}$$

Analogously, the same methodology can be applied to each term $\tilde{u}^\omega \cdot \tilde{h}^\omega$:

$$\min_{\tilde{h},\tilde{\pi},\tilde{p}\geq 0} \quad \sum_{\omega} [\ (\tilde{\beta}_0^{-,\omega} + \sum_{j=1}^{\tilde{m}} \tilde{\beta}_j^{-,\omega} \tilde{u}_j^\omega) \tilde{h}^\omega + H\tilde{\pi}^\omega + \sum_{j=0}^{\tilde{m}} \tilde{p}_j^\omega\ ] \tag{27}$$

$$\tilde{\pi}^\omega + \tilde{p}_j^\omega \geq \tilde{\beta}_j^{+,\omega} \tilde{u}_j^\omega \tilde{h}^\omega, \quad \tilde{\pi}^\omega + \tilde{p}_0^\omega \geq \tilde{\beta}_0^{+,\omega} \tilde{h}^\omega, \quad \forall j,\ \forall \omega \tag{28}$$

Let us define $\mathbf{u}_r^\omega \triangleq \beta_{r,0}^{-,\omega} + \sum_{j=1}^{m} \beta_{r,j}^{-,\omega} u_{r,j}^\omega$ and $\tilde{\mathbf{u}}^\omega \triangleq \tilde{\beta}_0^{-,\omega} + \sum_{j=1}^{\tilde{m}} \tilde{\beta}_j^{-,\omega} \tilde{u}_j^\omega$.

The robust counterpart of problem **MINLP-D** is the problem **MINLP-R**:

(MINLP-R) (29)

$$\min_{\substack{h,\tilde{h},\pi,p,\tilde{\pi},\tilde{p}\\ f,m,\lambda,\theta,y_o}} \sum_{\omega\in W}\sum_{r\in R(\omega)} \mathbf{u}_r^\omega h_r^\omega + \sum_{\omega\in W} \tilde{\mathbf{u}}^\omega \tilde{h}^\omega + \sum_{\omega\in W}\int_0^{\tilde{h}^\omega} (\log \frac{x}{\chi^\omega - x})dx$$
$$+ \sum_{\omega\in W}\sum_{r\in R(\omega)} \left(H\pi_r^\omega + \sum_{j=0}^{m} p_{r,j}^\omega \right) + \sum_{\omega\in W} \left(\tilde{H}\tilde{\pi}^\omega + \sum_{j=0}^{n} \tilde{p}_j^\omega \right)$$
$$\text{s.t.} \quad (1a), (1d), (1e), (5) - (20), (26), (28)$$

From now on, **MINLP** will be used to refer indistinctly to both **MINLP-D** and **MINLP-R** if such is the context.

5. Solution algorithm

We apply an outer-approximation algorithm for mixed integer non-linear optimization problems detailed in Floudas (1995), which is extracted from the work presented in Duran & Grossmann (1986). A summarized, simpler version of the notation is used for making easier the description of the algorithm.

- $\mathbf{y}$: Vector of integer variables whose components are: $f_\rho^{v,\omega}, f_\rho^{v,\emptyset}, m_\rho^k$, $\lambda^{v,o}$, $\theta_{i',i}^{k,o} \in \mathbb{Z}^+, \hat{y}_o \in \{0,1\}$ for **MINLP**.
- $\mathbf{x}$: Continuous variables. $\mathbf{x}$ corresponds to $h_r^\omega, \tilde{h}^\omega$ for **MINLP-D**, while $\mathbf{x}$ corresponds to $h_r^\omega, \pi_r^\omega, p_{r,j}^\omega, \tilde{h}^\omega, \tilde{\pi}^\omega, \tilde{p}_j^\omega$ for **MINLP-R**.
- $\mathcal{Y}$: Set containing values for $\mathbf{y}$ that verify constraints (6)-(16) plus (20) for **MINLP**. Actually, all constraints that involve only trains and railcars.
- X set. Constraints involving only continuous variables. (1a), (1d), (1e) and (19) for **MINLP-D**, also includes (26), (28) for **MINLP-R**.
- $g_\ell(\mathbf{x},\mathbf{y}) \le 0$, $\ell = 1,2,3$. Relationship between rail freight demand flows and flows of railcars and trains, i.e., constraints (5) for $\ell = 1$, (17) for $\ell = 2$ and (18) for $\ell = 3$, for **MINLP**.
- The objective function for **MINLP** will be denoted by $F(\mathbf{x})$.

The algorithm decomposes the original problem **MINLP** into one non-linear primal subproblem **NLPP** (30) :

$$\textbf{(NLPP)} \qquad \min_{\mathbf{x}\in X} F(\mathbf{x}) \tag{30}$$

$$g_\ell(\mathbf{x},\mathbf{y}^{(\mathbf{s})}) \le 0, \quad \ell = 1,2,3 \tag{30a}$$

$$\Rightarrow \mathbf{x}^* \longrightarrow \mathbf{x}^{(s}$$

and one mixed-integer linear master problem **MLMP** (31).

$$\textbf{(MLMP)} \quad \min_{\mathbf{x},\mathbf{y},z} z \tag{31}$$

$$z \ge F(\mathbf{x}^{(s)}) + \nabla F(\mathbf{x}^{(s)})(\mathbf{x}-\mathbf{x}^{(s)}), \quad \forall s \tag{31a}$$

$$g_\ell(\mathbf{x},\mathbf{y}) \le 0, \ \forall \ell, \quad \mathbf{x}\in X, \quad \mathbf{y}\in\mathcal{Y} \tag{31b}$$

$$z^{(s} \le z < UBD \tag{31c}$$

$$\Rightarrow \quad z^*,\mathbf{x}^*,\mathbf{y}^* \longrightarrow z^{(s+1},\hat{\mathbf{x}},\mathbf{y}^{(s+1}$$

MLMP includes two type of cuts induced by $\mathbf{x}^{(s}$, $\forall s$: a linearization around $\mathbf{x}^{(s}$ of the convex functions $F(\mathbf{x})$ (32):

$$z \ge F(\mathbf{x}^{(s)}) + \nabla F(\mathbf{x}^{(s)})(\mathbf{x}-\mathbf{x}^{(s)}), \ \forall s \tag{32}$$

and $g_\ell(\mathbf{x},\mathbf{y})$ (33):

$$0 \ge g_\ell(\mathbf{x}^{(s},\mathbf{y}) + \nabla g_\ell(\mathbf{x}^{(s},\mathbf{y})(\mathbf{x}-\mathbf{x}^{(s)}), \ \forall s, \ \ell = 1,2,3 \tag{33}$$

In this case, $g_\ell(\mathbf{x},\mathbf{y})$ are all linear functions, so cuts of the type (33) are equivalent to $g_\ell(\mathbf{x},\mathbf{y}) \le 0$.

Subproblem **NLPP** generates an upper bound on the **MINLP** solution by fixing the value of the integer variables and solving the resulting **MINLP**, while solving **MLMP** allows to obtain a lower bound. **MLMP** results as an outer linearization of the **MINLP** non-linear objective function and constraints at $\mathbf{x}^{(s}$. **NLPP** provides a temptative value $\mathbf{x}^{(s}$ for the continuous variables $\mathbf{x}$ at iteration $(s$, while the solution of **MLMP** provides the new values for the integer variables, to solve a new iteration of **NLPP**. Observe that solution $\mathbf{x}^*,\mathbf{y}^*$ verifies (31b), that is, **NLPP** is feasible.

NLPP is a problem with non-linear objective function and linear constraints. It can be observed that, were it not for constraints $g_2 \le 0$ in (30a) (that is, (17) evaluated at $\mathbf{y}^{(\mathbf{s})}$), **NLPP** could be decomposed by $\omega \in W$. The objective function terms are also separable by ω. This condition allows decomposing **NLPP** into a set of non-linear subproblems, one for each $\omega \in W$, after applying a Lagrangian relaxation on constraints $g_2 \leq 0$ in (30a).

Also, the algorithm requires to obtain an initial feasible solution. We have opted by directly solving **MINLP** without any objective function, under condition that a minimum demand is transported by rail. This condition avoids the simplest solution, with all demand transported by truck, which is not a valid solution for the problem **MINLP**.

The convergence of the method relies on the characteristics of the functions and sets which define the problem ((Duran & Grossmann, 1986, Theorem 3)). In short, these conditions are the following:

- X is a non-empty compact and convex set;
- the function $F(\mathbf{x})$ is convex and once continuously differentiable, and functions $g_\ell(\mathbf{x}, \mathbf{y}), \ell = 1, 2, 3$ are convex in $\mathbf{x}$ and once continuously differentiable,
- the set $\mathcal{Y}$ is a finite discrete set, and finally
- a constraint qualification holds for each **NLPP** problem, given that $g_\ell(\mathbf{x}, \mathbf{y}), \ell = 1, 2, 3$ and constraints that defines X are all linear.

he algorithms applied to solve **MINLP**, and **NLPP** and its subproblems involved are detailed in Appendix E.

6. Computational results

The model was implemented using Python 3, and the solvers *optimize* from Scipy and CPLEX V12.7. Tests were carried out on a R5500 workstation using Intel® Xeon® CPU 5645 with 2.40 GHz and 48 Gb RAM. The analysis of results was conducted in R. Tests are centered on the Trans-European Transport Network (TEN-T). Figure 2 shows a schema of the lines used in the tests that cover the region, from Valencia and Zaragoza (Spain) on the south-west to Malaszewicze (Poland) on the north-east, and from Marseilles (France) and Milan (Italy) to Rotterdam (the Netherlands) and Hamburg (Germany) on the north. The rail network has $17,406$ km with a maximum train length from 350 m. to 750 m. The maximum weight that trains can transport varies from 550 to $1,100$ tons.

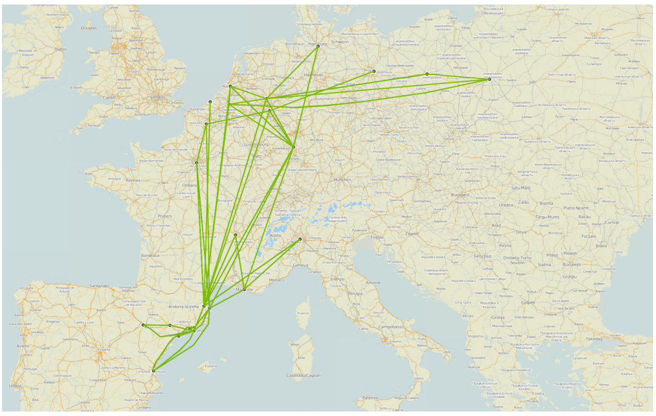


Fig. 2. Lines used for tests

6.1. Data preparation

Data preparation for the tests has followed four stages: a) selection of products and associated OD-pairs, b) selection of factors that determine disutilities, c) estimation of significant parameters of a logit based RUM model and d) estimation of additional parameters. Data preparation details and data sources appear described in Appendix F.

Regarding the factors for disutilities, three variables related to the trip characteristics were finally chosen, providing the best RUM model: a) distance, b) the difference between train price and road price, and c) GHG-emissions. A dummy variable for each type of product transported was added: a 0-1 value for capturing special characteristics for each product. Details can be found in Appendix G

The volume transported was calculated as a fraction of the total demand transported by train and truck, during 2018, for the products and regions selected. The fraction varies from 20% and 70%, depending on the product and its origin or destination. The total volume transported in the period is $7,764,760$ tons, distributed in Chemical products (42%), Fruits and Vegetables (27%), Grain (13%), Steel and Iron (8%), Vehicles (8%), and Automotive complements (3%).

A logit approximation was applied to estimate the values for the β-parameters, by using the R-package *mlogit* (Croissant (2020)). A common approximation for all OD-pairs was made. Different tests were performed to validate the quality of the estimated coefficients: the marginal effects of the continuous parameters for each product and the capability to reproduce

Table 1: Problem size for tests with several Carriers.

N	T	Y	A	W	Γ	R	$\mathcal{V}$	K	O	Variables	Int.	Bin.	Rows
95	20	34	266	115	140	240	3	3	5	$4,013/8,997$	$3,516$	5	$4,258/8,750$

the observed flows, with a high value of the coefficient of determination R^2, equal to 0.99. Details regarding the analysis of the RUM model can be found in Appendix G.

6.2. Description of the tests

Different groups of tests were executed to check the model utility and its efficiency. A combination of three criteria was used to define these groups. The first criterion takes into account whether exists or not carrier competition on rail freight transport. A third of the tests simulate the situation where only one carrier operates the rail freight network, acting like a monopoly. In contrast, the other two-thirds of tests correspond to a "Carrier Competition" analysis, where different carriers operate under competition. The second criterion is based on the robustness level applied. The 0-level, where no robustness is applied, is equivalent to a deterministic case. In this case, the β-parameters are based on their average value. The level number indicates the maximum number of β-parameters that are allowed to divert from its average value, taking a value from the interval $[\beta^- - \beta^+, \beta^- + \beta^+]$. The third criterion affects only the "Carrier Competition" cases, defining two types of tests: a) those with a previously fixed allocation of slots for each carrier and b) tests where the number of slots is left variable and determined by the model, thus making possible to get a modal split closer to the a priori utilities of the RUM model. Two groups of acronyms characterize the tests: first, **CF**, **CD** and **M** apply for the carrier competition cases with fixed allocation (**CF**), carrier competition cases with variable allocation of slots (**CD**), and the monopoly situation (**M**). Second, **Det**, **RL 1**, **RL 2** and so on, label tests depending on the level of robustness applied. **Det** corresponds to the Deterministic version of the model. Due to lack of space, only some cases are reported. Table 1 shows the size of the sets and the problem size for *CF* and *CD* tests. The first value for **Variables** and **Rows** columns corresponds to robustness level 0 or **Det** tests, while the second is for the robust version of the tests. The number of integer variables (**Int.** column) and binary variables (**Bin.** column) is the same for all the tests.

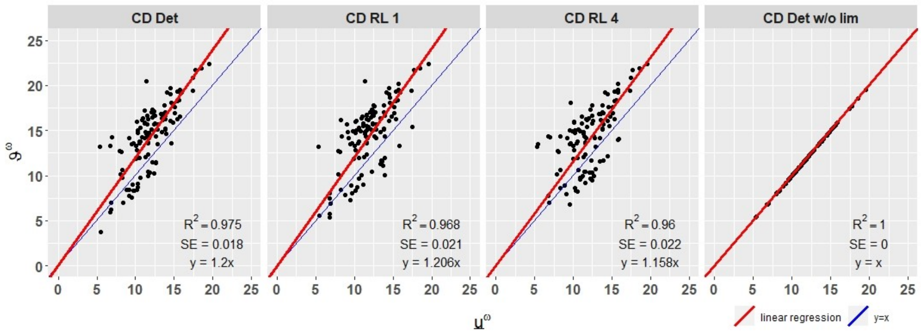


Fig. 3. Comparison between $\underline{u}^\omega$ and ϑ^ω values

6.3. Modal split compliance

In Section 3 the modal choice properties of the model are detailed. The modal split behavior, as appears in equation (4), depends on two parameters: $\tilde{u}^\omega$ and ϑ^ω. The first one corresponds to road utility function, while the second one does not exactly match the train utility: the Lagrange multipliers associated to the constraints that condition the way products are transported by train exert some influence on the modal split. Whether this influence is strong or weak, it mainly depends on how the right hand terms tighten the different constraints, once calculated the solution to the optimization problem. In our model, the constraints that mainly put pressure are those which are related with infrastructure capacity (10), (11) and (14), rolling stock capacity (15) and (16), and cost-effectiveness for carriers (17) and (18). From (4), $\vartheta^\omega = \tilde{u}^\omega - \log\left(\chi^\omega/\tilde{h}^\omega - 1\right)$, and let $\underline{u}^\omega = \min_{r\in R(\omega)} u_r^\omega$ be an approximation to ϑ^ω as expressed in (3). $u^\omega, \tilde{u}^\omega$ are the utilities used in the experiments, and for each $\omega \in W$, $\tilde{h}^\omega/\chi^\omega$ corresponds to the road share derived form the solution obtained.

Figure 3 plots the relationship of $\underline{u}^\omega$ versus ϑ^ω for different examples based on the **CD**-cases. The graph on the left corresponds to the Deterministic (**Det**) test, while the next two graphs show the **RL 1** and **RL 4** tests. The experiment corresponding to the graph on the right, named **CD Det w/o lim**, is based on **CD Det**-test, although with constraints (10), (11) (14), (15), (16) , (17) and (18) relaxed. The main linear regression indicators are displayed on each graph (R^2, the standard error SE and the x-coefficient). As can be seen, $\underline{u}^\omega$ and ϑ^ω values are perfectly correlated for the **CD Det w/o lim** solution, following the line $y = x$, but for the **CD Det**, **CD RL 1** and **CD RL 4** solutions, the constraints that are active

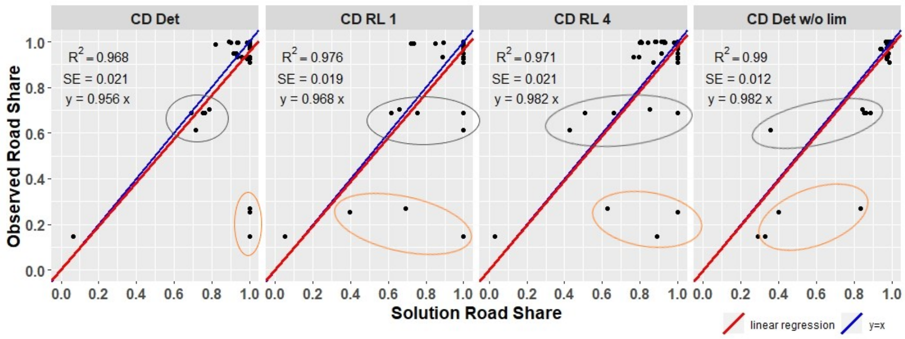


Fig. 4. Comparison between the solution road share and the observed road share

alter the expected value for ϑ^{ω}. Although the three graphs are very similar, these examples show that dispersion slightly increases with the robustness level.

6.4. Results of the tests

Figure 4 illustrates the goodness of fit of the model by comparing the road share that outcomes from the solution, and the observed road share, for the **CD Det**, **CD RL 1** and **CD RL 4** tests, and also, for the **CD w/o lim** example. All graphs compare both values directly by plotting one versus the other. Note that the vertical axis values (the observed values) are the same for all the graphs, while the horizontal axis values correspond to each test's solution. The grouped points, highlighted with two different colors, correspond to the same origin-destination-products triples for all tests. For the yellow group, a better prediction regarding the **Det** test is obtained when applying some level of robustness. In contrast, for the gray group, the **Det**-test solution provides a more accurate prediction. The fact that the **CD Det w/o lim**-test solution has outliers (and the **Det** test gives a better prediction for some of them) illustrates the influence that railway conditions have on modal split when road and train compete.

Table 2 summarizes the algorithm performance. As before, the first two columns identify the test. Column **rel. error** shows the relative error when the algorithm stops. Column **number it tot** shows the total number of iterations for solving the full problem **MINLP**, while column **number it NLPP** shows the average number of iterations used to solve the primal sub-problem **NLPP**. The next four columns correspond to CPU consumption in seconds. Column **cpu MINLP** shows the total CPU used to solve **MINLP**.

Table 2: Algorithm performance: relative error, iterations, cpu consumption.

case	rob level	rel error	number iter. MINLP	number iter. NLPP	cpu (seconds) MINLP	cpu (seconds) it	cpu (seconds) NLPP	cpu (seconds) MLMP
CF	Det	1.9e-5	36	24	87	2.32	1.44	0.88
	RL 1	2.7e-5	34	23	262	7.58	6.66	0.92
	RL 4	1.3e-5	36	22	243	6.65	6.04	0.60
CD	Det	2.9e-5	35	21	200	5.59	1.13	4.46
	RL 1	1.1e-5	35	25	285	8.02	7.21	0.81
	RL 4	1.8e-5	41	20	279	6.70	5.13	1.56
M	Det	0.8e-5	42	5	232	5.45	0.33	5.11
	RL 1	0.7e-5	41	5	196	4.68	0.99	3.69
	RL 4	1.1e-5	36	5	62	1.61	0.92	0.68

Column **cpu it** corresponds to the average CPU-consume per iteration, and it is decomposed on the next two columns: CPU-use required by the primal subproblem **NLPP** (column **NLPP**) and the CPU consumed to solve the master problem **MLMP** (column **MLMP**). As can be seen, the algorithm is quite fast and efficient, allowing to solve the different experiments in less than five minutes. A relevant CPU increase in robustness cases appears when different carriers compete against each other, mainly related to the CPU-time required to solve **NLPP**.

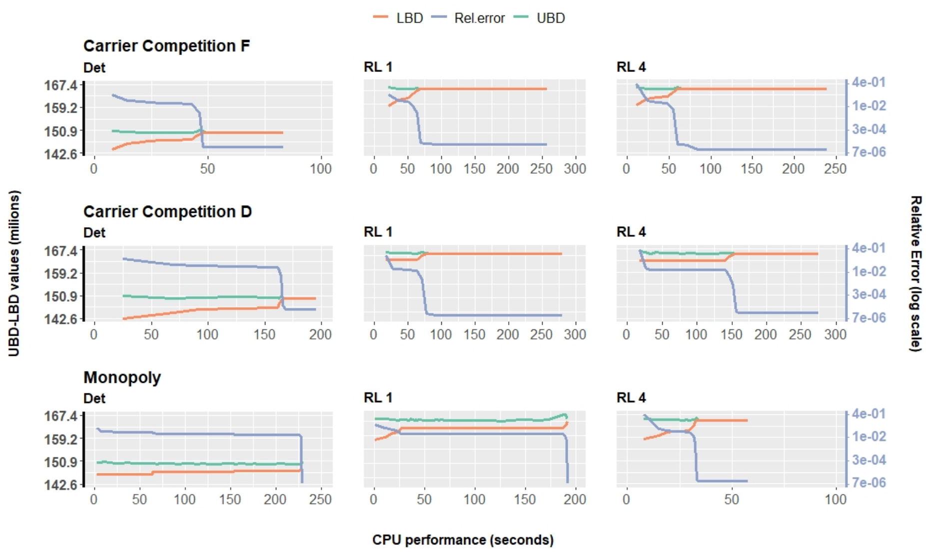


Fig. 5. UBD vs LBD, and alg. relative error evolution.

Figure 5 shows the upper bound, the lower bound and the relative error (in logarithmic scale) evolution for the algorithm to solve **MINLP**. The

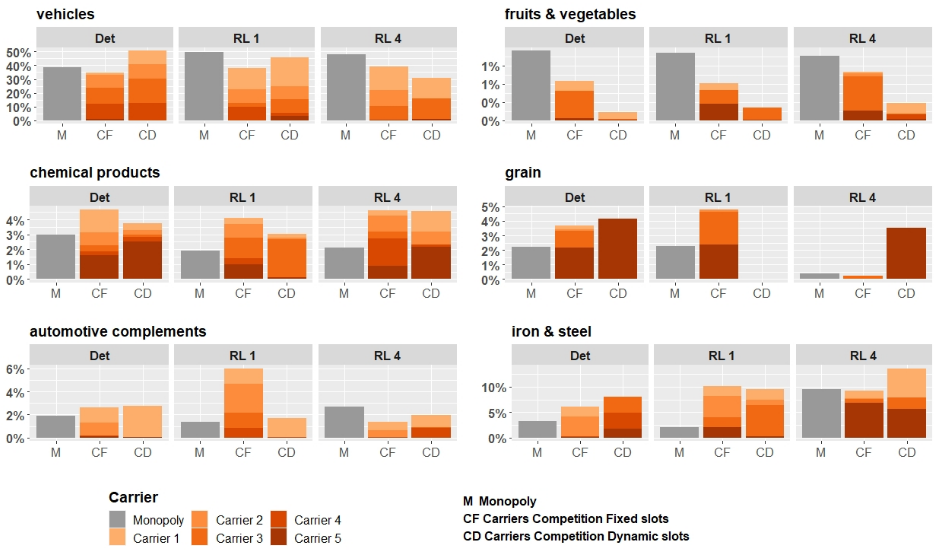


Fig. 6. Volume Modal Share. By products, different robustness levels

y-axis on the left corresponds to the upper bound and lower bound values (expressed in millions), while the y-axis on the right, in blue, shows the relative error values. All the graphics share the same scale on both y-axis. The x-axis represents the CPU consumption in seconds. The first row of graphics corresponds to **CF**-tests, the second row shows the algorithm evolution for **CD**-tests, and the third row for the **M**-tests.

Finally, a few examples of the information about the carrier's operation the model can provide. Figure 6 shows the carrier share and the monopoly share for each product and each test. The range of oranges represents the carriers, while the gray color corresponds to the monopolistic situation. In most cases, when comparing the **CF** and **CD** results, there is a better distribution among carriers in the **CF** experiments than in the **CD** experiments. This behavior is due mainly to the initial slots allocation. While the **CD** situation allows one or few carriers to gather the whole train transport easily, the **CF** situation limits more clearly the demand each carrier can transport. Concerning the modal share, per volume and import, there is barely any difference among the tests, being relatively small for rail freight, as usual. Experiments give a train share between 4% and 6% in volume and only a 3% in import. Both percentages are coherent with the observed data.

7. Conclusion and future research

This paper presents a combined modal-split/traffic assignment model for rail and road freight transport, with detailed modeling of the various railway traffic flows (e.g., railcars either full or empty, volumes of newly formed trains at yards...) for multi-operator scenarios where the modal split has to be applied. The model is formulated as a non-linear integer optimization problem following the classical relative entropy function maximization. The model accounts for the large variability that the utility coefficients may have for reasons such as difficulties in the data collection and the predominant role of the road mode of transport. To this end, a robust counterpart of the model is formulated to take into account more conservative modal splits under a limited worst-case standpoint. An algorithm based on the outer approximation method is developed to provide accurate solutions in a reasonable computational time for both the robust and non-robust models.

Examples centred on a section of the Trans-European Transport Network, the TEN-T Core network corridors, are reported to test the model's applicability. Results show that this model can be a helpful tool for analysing the possible shippers' response to the different railway carriers' services competing with each other as well as scenarios where (implicit) capacity limitations in the scenarios to be evaluated may necessarily be taken into account.

The model can be the object of future extensions such as including more modes (e.g., inland waterways transport) in a multimodal framework. Also, the assignment component of the model can be extended by including non-linearities under a variational inequalities formulation.

Acknowledgement

This research is supported by Grant TRA2016-76914-C3-1-P of the Spanish Ministerio de Economía y Competitividad. We would like to thank Ricardo García, Full Professor at Universidad de Castilla la Mancha and Luis Cadarso, Associate Professor at Universidad Rey Juan Carlos, for their valuable suggestions and comments. We would also like to thank three anonymous referees for their feedback and useful comments.

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Appendix A. Sets, Parameters, and Variables Summary.

Table A.3: List of sets

$\mathcal{O}$	carriers	$Y(o)$	yards where carrier $o \in \mathcal{O}$ operates
A	directed arcs	$\mathcal{V}(\rho)$	railcars compatibles with ρ-line
Y	yards	$R(\omega)$	t-paths from origin $\mathfrak{o}(\omega)$ to destination $\mathfrak{d}(\omega)$. $R = \cup_{\omega \in W} R(\omega)$
T	terminals	$R(\rho)$	t-paths which contains line ρ
W	OD-pairs and product	$R(\omega, \rho)$	t-paths from origin $\mathfrak{o}(\omega)$ to destination $\mathfrak{d}(\omega)$ containing line ρ
Γ	carriers' lines	$R(\omega, o)$	carrier $o \in \mathcal{O}$ t-paths for OD-pair in ω
$\mathcal{V}$	railcars	$\Gamma(o)$	lines of carrier $o \in \mathcal{O}$
K_M	locomotive types	$\Gamma(a, o)$	lines of carrier $o \in \mathcal{O}$ containing arc a
		$\Gamma(v, o)$	lines of carrier $o \in \mathcal{O}$ compatible with railcars of type $v \in \mathcal{V}$
	$\Gamma_i^+(o)/\Gamma_i^-(o)$	$(\Gamma_i^+(v, o)/\Gamma_i^-(v, o))$	- lines of carrier $o \in \mathcal{O}$ outgoing from/incident to i-yard (also compatible with v-type railcars)

Table A.4: List of parameters.

parameter	description
$\mathcal{T}$	- period of the study (for instance, a year expressed in hours)
$\bar{\mathcal{T}}$	- effective time rolling stock runs during the period of the study $\mathcal{T}$ (for instance, total effective hours available for a year)
χ^ω	- total demand for $\mathfrak{p}(\omega)$-product and origin-destination pair $(\mathfrak{o}(\omega), \mathfrak{d}(\omega))$.
$u_r^\omega, \tilde{u}^\omega$	- generalized cost for OD-pair and unit of product ω, for train and truck, respectively.
$\alpha^{v,\mathfrak{p}(\omega)}$,$\alpha^v, \ell^v$	- capacity per unit of product $\mathfrak{p}(\omega)$ on railcar of type v / tare/length of v-type railcar.
$\bar{\ell}_\rho$	- maximum train length allowed on line ρ.
$\bar{\alpha}_\rho^k$	- maximum weight allowed for locomotive of type k on line ρ.
$N_\rho, N_a, \tilde{N}_i$	- maximum train capacity per line ρ, arc a and yard i, respectively.
$L^{v,o}, \tilde{L}^{k,o}$	- maximum number of railcars of type v and locomotive of type k that carrier o may have available, respectively
t_ρ	- the average run time for one train in line ρ
U_r^ω	- price per $\mathfrak{p}(\omega)$-unit paid by shipper when transported by train from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ on carrier path r.
$C_i^{k,o}, \tilde{C}_i^{k,o}$	- cost for train formation/decomposition at yard i.
$\hat{C}_\rho^k$	- travel cost of k-train when runs on path ρ.
$D^{v,o}$	- o-carrier cost for renting and/or maintenance of v-railcars.

Table A.5: List of variables

All of them are non-negative. B: binary - I: integer - C: continuous

variable		description
h_r^ω	C	- total tons of product $\mathfrak{p}(\omega)$ transported from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ by train, on t-path r.
$\tilde{h}^\omega$	C	- total tons of product $\mathfrak{p}(\omega)$ transported from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ by road.
m_ρ^k	I	- total number of locomotives of type $k \in K_M$ that run on $\rho \in \Gamma$.
$m_{\rho,i}^k$	I	- total number of locomotives of type k that run on $\rho \in \Gamma$ and stops at yard $i \in Y$.
$f_\rho^{v,\omega}$	I	- total number of loaded railcars of type v that transport product $\mathfrak{p}(\omega)$ from $\mathfrak{o}(\omega)$ to $\mathfrak{d}(\omega)$ using $\rho \in \Gamma$.
$f_\rho^{v,\emptyset}$	I	- total number of empty railcars of type $v \in \mathcal{V}$ running on $\rho \in \Gamma$.
F_ρ^v	I	- total number of railcars (empty and loaded) of type $v \in \mathcal{V}$ running on $\rho \in \Gamma$. $F_\rho^v = f_\rho^{v,\emptyset} + \sum_{\omega \in W} f_\rho^{v,\omega}$
$\theta_{i',i}^{k,o}$	I	- total number of locomotives of type k, owned by carrier o, that run from yard i' to yard i.
$\lambda^{v,o}$	I	- minimum number of railcars of type v needed for carrier o to provide service.
$\hat{y}^o$	B	- binary variable to avoid infeasibility due to relationship between price and cost.
$\pi_r^\omega, p_{r,j}^\omega$, $\tilde{\pi}^\omega, \tilde{p}_j^\omega$	C	- auxiliary variables for the robust version of the model.

Appendix B. Modal choice properties of the model.

The modal choice properties of the model will be analysed in detail in this section. Let us remember the notation used for the formulation of the problem. Variables h_r^ω, $\tilde{h}^\omega$ are the total flow transported by train using t-path $r \in R(\omega)$ and truck, respectively, for an OD-pair and product represented by the triplet ω. Also, we have defined the flow vectors $\mathbf{h}^\omega = (..., h_r^\omega, ...)^\top \in \mathbb{R}^{|R(\omega)|}$, $\omega \in W$, $\mathbf{h} = (..., \mathbf{h}^\omega, ...)^\top \in \mathbb{R}^{|W|}$ and $\tilde{\mathbf{h}} = (..., \tilde{h}^\omega, ...)^\top \in \mathbb{R}^{|W|}$. Parameters $\tilde{u}^\omega, u_r^\omega$ are the generalized cost or disutility, for OD-pair and product ω, when transported by truck and by train using t-path $r \in R(\omega)$, respectively. Variables related to flow of railcars, locomotives, flow of trains between yards and other auxiliary variables are assumed to be comprised in a generic vector of variables $\mathbf{y}$ lying in a specific domain $\mathcal{Y}$. Finally, variables $\mathbf{h}, \tilde{\mathbf{h}}$ and $\mathbf{y}$ will be related each other by some binding constraints $g_\ell(\mathbf{h}, \mathbf{y}) \leq 0,\ \ \ell = 1, ..., m$.

The model is formulated as the following non-linear integer optimization problem, as it appears in Section 3:

$$\min_{\mathbf{h},\tilde{\mathbf{h}},\mathbf{y}} \quad F(\mathbf{h},\tilde{\mathbf{h}}) = \sum_{\omega\in W}\left[\sum_{r\in R(\omega)} u_r^\omega h_r^\omega + \int_0^{\tilde{h}^\omega} G_\omega^{-1}(s)ds\right] \tag{1}$$

$$\text{s.t.} \quad \sum_{r\in R(\omega)} h_r^\omega + \tilde{h}^\omega = \chi^\omega \qquad \omega \in W \tag{1a}$$

$$g_\ell(\mathbf{h},\mathbf{y}) \leq 0 \qquad \ell = 1,..,m \tag{1b}$$

$$\mathbf{y} \in \mathcal{Y} \tag{1c}$$

$$h_r^\omega \geq 0, \qquad \omega \in W, \tag{1d}$$

$$\tilde{h}^\omega \geq 0, \qquad \omega \in W,\ r \in R(\omega) \tag{1e}$$

It is aimed to reflect shippers priorities, as well as the modal split behavior. Then, following the models for user equilibrium with variable demand developed in Sheffi (1985), the problem is expressed using the excess-demand formulation, being $G_\omega^{-1}(\cdot)$ the inverse demand function, as expressed in (B.1) :

$$G_\omega^{-1}(\tilde{h}^\omega) = \tilde{u}^\omega + \log\left(\frac{\tilde{h}^\omega}{\chi^\omega - \tilde{h}^\omega}\right), \quad \omega \in W \tag{B.1}$$

corresponding to the direct demand function $G_\omega(\cdot)$ for the road mode of transportation, that provides the amount of flow $\tilde{h}^\omega$ transported by road

$$\tilde{h}^\omega = G_\omega(u^\omega) = \chi^\omega \left\{1 + \exp(\tilde{u}^\omega - u^\omega)\right\}^{-1} \tag{B.2}$$

In (1), the first component corresponds to total generalized cost for OD-pair and product, and the second component represents the total generalized cost for the excess demand transported by truck, for OD-pair and product. The detailed expression for the excess-demand component of (1) developed in (B.3) allows to guarantee having a convex objective function:

$$\begin{aligned}\int_0^{\tilde{h}^\omega} G_\omega^{-1}(s)ds &= \int_0^{\tilde{h}^\omega}\left(\tilde{u}^\omega + \log\left(\frac{s}{\chi^\omega - s}\right)\right)ds \\ &= \tilde{u}^\omega\tilde{h}^\omega + \int_0^{\tilde{h}^\omega}\log\left(\frac{s}{\chi^\omega - s}\right)ds = \\ &= \tilde{u}^\omega\tilde{h}^\omega + \tilde{h}^\omega\log(\tilde{h}^\omega) + (\chi^\omega - \tilde{h}^\omega)\log(\chi^\omega - \tilde{h}^\omega) - \chi^\omega\log(\chi^\omega)\end{aligned} \tag{B.3}$$

Then, the objective function (1) results as follows:

$$F(\mathbf{h},\tilde{\mathbf{h}}) = \sum_{\omega\in W}\sum_{r\in R(\omega)} u_r^\omega h_r^\omega + \sum_{\omega\in W}\tilde{u}^\omega\tilde{h}^\omega + \sum_{\omega\in W}\int_0^{\tilde{h}^\omega}\log\left(\frac{s}{\chi^\omega - s}\right)ds \tag{B.4}$$

The modal choice properties of the model derive from the following first order conditions of problem (1) with respect the variables h_r^ω, $\tilde{h}^\omega$:

$$\frac{\partial F}{\partial h_r^\omega} = u_r^\omega = \vartheta^\omega - \gamma_r^\omega + \xi_r^\omega, \qquad \xi_r^\omega \geq 0, \;\; \xi_r^\omega h_r^\omega = 0 \tag{B.5a}$$

$$\frac{\partial F}{\partial \tilde{h}^\omega} = \tilde{u}^\omega + \log\left(\frac{\tilde{h}^\omega}{\chi^\omega - \tilde{h}^\omega}\right) = \vartheta^\omega + \eta^\omega, \qquad \eta^\omega \geq 0, \; \eta^\omega \tilde{h}^\omega = 0 \tag{B.5b}$$

where ϑ^ω, ξ_r^ω and η^ω are the Lagrange multipliers of constraints (1a), (1d) and (1e), respectively. Also, γ_r^ω result from the Lagrange multipliers ζ_ℓ of constraints (1b) as

$$\gamma_r^\omega = \sum_{g_\ell(\mathbf{h},\mathbf{y})=0} \zeta_\ell \frac{\partial g_\ell}{\partial h_r^\omega} \tag{B.6}$$

From (B.5a) and being $\xi_r^\omega \geq 0$:

$$\vartheta^\omega \leq u_r^\omega + \gamma_r^\omega, \;\; \forall r \in R(\omega), \forall \omega \in W \tag{B.7}$$

It must be remarked that, because Lagrange multipliers η^ω must be finite, any solution of previous problem (1) must verify that $\tilde{h}^\omega > 0$ and $\tilde{h}^\omega < \chi^\omega$. Thus, from (1a), $\sum_{r\in R(\omega)} h_r^\omega > 0$, $\forall \omega \in W$, and then:

$$\begin{aligned}
&\forall \omega \in W, \; \sum_{r\in R(\omega)} h_r^\omega > 0 \text{ and } h_r^\omega \geq 0 \;\; \forall r \in R(\omega) && \Longrightarrow \\
&\forall \omega \in W, \; \exists r \in R(\omega), \; h_r^\omega > 0 \text{ and } \xi_r^\omega = 0 && \Longrightarrow \\
&\forall \omega \in W, \; \exists r \in R(\omega), \; \vartheta^\omega = u_r^\omega + \gamma_r^\omega
\end{aligned} \tag{B.8}$$

Then, from (B.7) and (B.8):

$$\vartheta^\omega = \min_{r\in R(\omega)} \{u_r^\omega + \gamma_r^\omega\}, \;\; \omega \in W \tag{B.9}$$

From (B.5b), taking into account that $\tilde{h}^\omega > 0 \implies \eta^\omega = 0$, $\forall \omega \in W$, the modal split following a logit model can be derived after some calculation:

$$\frac{\tilde{h}^\omega}{\chi^\omega} = \{1 + \exp(\tilde{u}^\omega - \vartheta^\omega)\}^{-1} \tag{B.10}$$

Appendix C. Costs associated with rail freight transport.

In this section we will detail the costs we have applied in the tests, and their relationship with the parameters on the constraints (17).

- Costs per km-train. All of them are defined per track, based on its length, and from tracks, assigned to ρ-path as a sum of costs. They result in parameter

$\hat{C}^k_\rho$:

- Annual driver salary divided by the average total amount of km per driver.
- Annual locomotive maintenance divided by the average total amount of km per locomotive.
- Annual amortisation, financial and assurance costs: all of them divided by the average total amount of km per locomotive.
- Energy supplied by the Infrastructure Manager. It is usually charged per km.
- Fee for use of the infrastructure. It is usually charged per km, sometimes depending on other factors, as the type of track or type of train.

- Costs per train. All of them are defined per track and from tracks, assigned to ρ-path as a sum of costs. They are added to parameter $\hat{C}^k_\rho$ when corresponds:
  - Fee for running on particular tracks, as can be the Perthus tunnel, on Spain-France border.
  - Fee for changes on locomotives or railcars, when traversing zones of different track characteristics or electrification, for instance.
- Costs per railcar. They are an annual amount per railcar. They correspond to the parameter $D^{v,o}$:
  - Annual maintenance
  - Annual amortisation and financial costs.
- Costs for composition and decomposition of trains. All of them are defined per train and yard.
  - Train composition. Includes shunting movements. It corresponds to parameter $C^{k,o}_i$.
  - Train decomposition. Includes shunting movements and train control before departure. It corresponds to parameter $\bar{C}^{k,o}_i$

Appendix D. Details for Robustness Formulation.

In this section, we will explain in detail how robustness is applied in the utility function. First of all, let us remember the meaning of the elements we need for the robustness formulation. Let h^ω_r be the total demand during period $\mathcal{T}$, or flow, transported by train for OD-pair and product ω using t-path r, and let $\tilde{h}^\omega$ be the total demand transported by truck, for OD-pair and product ω. We assume that the systematic component of the disutilities for the rail and road transport modes are given by affine functional forms of m and $\tilde{m}$ explanatory variables as in

(D.1). Typically these explanatory variables are travel time, price, distance, GHG (Greenhouse Gas) emissions, among others.

$$u_r^\omega = \beta_0^\omega + \sum_{j=1}^{m} \beta_j^\omega u_{r,j}^\omega, \qquad \tilde{u}^\omega = \tilde{\beta}_0^\omega + \sum_{j=1}^{\tilde{m}} \tilde{\beta}_j^\omega \tilde{u}_j^\omega \tag{D.1}$$

We assume we can obtain reasonable estimates for the utility function parameters' mean value and confidence intervals. From them, the uncertainty of parameters β may be expressed as follows:

$$\beta_j^\omega \in [\beta_j^{-,\omega} - \beta_j^{+,\omega}, \beta_j^{-,\omega} + \beta_j^{+,\omega}],\ j = 0,\dots,m, \quad \forall \omega \in W \tag{D.2}$$

$$\tilde{\beta}_j^\omega \in [\tilde{\beta}_j^{-,\omega} - \tilde{\beta}_j^{+,\omega}, \tilde{\beta}_j^{-,\omega} + \tilde{\beta}_j^{+,\omega}],\ j = 0,\dots,\tilde{m}, \quad \forall \omega \in W \tag{D.3}$$

Here, we will analyse the case for the uncertainty in u_r^ω. Given the similarity between u_r^ω and $\tilde{u}^\omega$ composition, the results for the former can be applied to the latter. For simplicity, we remove the r and ω indexes. Let us define the uncertain set as follows:

$$\mathcal{B}(H) = \{\beta \in \mathbb{R}^{m+1} : \beta_j = \beta_j^- + \beta_j^+ \cdot z_j,\ j = 0,\dots,m,\ z \in \mathcal{Z}(H)\} \tag{D.4}$$

$$\mathcal{Z}(H) = \{z \in \mathbb{R}^{m+1} : |z_j| \leq 1,\ j = 0,\dots,m,\ \sum_{j=0}^{m} |z_j| \leq H\} \tag{D.5}$$

The following equivalences can be stated:

$$uh \Leftrightarrow (\sum_{j=0}^{m} \beta_j u_j)h,\ \beta \in \mathcal{B}(H) \Leftrightarrow \max_{z \in Z(H)} \{(\sum_{j=0}^{m} (\beta_j^- + \beta_j^+ z_j) u_j) h\}$$
$$\Leftrightarrow (\sum_{j=0}^{m} \beta_j^- u_j) h + \max_{z \in Z(H)} \{(\sum_{j=0}^{m} \beta_j^+ u_j z_j) \cdot h\}$$

Let $\mathcal{A}(H, h) = \max_{z \in Z(H)} \{(\sum_{j=0}^{m} \beta_j^+ u_j \cdot z_j) \cdot h\}$. Given $h^\star$, Koster et al. (2013) show that $\mathcal{A}(H, h^\star)$ is equivalent to the optimization problem:

$$\begin{aligned} \max_{z} \quad & (\sum_{j=0}^{m} \beta_j^+ u_j z_j) \cdot h^\star \\ \text{s.t.} \quad & \sum_{j=0}^{m} z_j \leq H, \quad 0 \leq z_j \leq 1,\ j = 0,\dots,m \end{aligned} \tag{D.6}$$

The dual of problem (D.6) can be stated as follows:

$$\begin{aligned} \min_{\pi,p} \quad & H\pi + \sum_{j=0}^{m} p_j \\ \text{s.t} \quad & \pi + p_j \geq \beta_j^{+} u_j h^{\star}, \quad \pi \geq 0, p_j \geq 0, \quad j = 0, \dots, m \end{aligned} \tag{D.7}$$

Then, we can reformulate the problem by replacing $u{\cdot}h$ by a new expression and adding a new set of constraints (all the indexes of the variables are now included):

$$\min_{\pi,p} \quad (\sum_{j=0}^{m} \beta_{r,j}^{-,\omega} u_{r,j}^{\omega}) h_r^{\omega} + H\pi_r^{\omega} + \sum_{j=0}^{m} p_{r,j}^{\omega} \tag{D.8}$$

$$\pi_r^{\omega} + p_{r,j}^{\omega} \geq \beta_{r,j}^{+,\omega} u_{r,j}^{\omega} h_r^{\omega}, \qquad \forall j,\ \forall \omega,\ \forall r \in R(\omega) \tag{D.9}$$

$$\pi_r^{\omega} \geq 0,\ p_{r,j}^{\omega} \geq 0, \qquad \forall j,\ \forall \omega,\ \forall r \in R(\omega) \tag{D.10}$$

That is, expression (D.8) replaces $u \cdot h$ in the objective function, and (D.9)-(D.10) should be added to the problem's set of constraints. Analogously, the same reasoning can be applied to $\tilde{u} \cdot \tilde{h}$:

$$\min_{\tilde{\pi},\tilde{p}} \quad (\sum_{j=0}^{\tilde{m}} \tilde{\beta}_{j}^{-,\omega} \tilde{u}_{j}^{\omega}) \tilde{h}^{\omega} + H\tilde{\pi}^{\omega} + \sum_{j=0}^{\tilde{m}} \tilde{p}_{j}^{\omega} \tag{D.11}$$

$$\tilde{\pi}^{\omega} + \tilde{p}_j^{\omega} \geq \tilde{\beta}_j^{+,\omega} \tilde{u}_j^{\omega} \tilde{h}^{\omega}, \qquad \forall j,\ \forall \omega \tag{D.12}$$

$$\tilde{\pi}^{\omega} \geq 0,\ \tilde{p}_j^{\omega} \geq 0, \qquad \forall j,\ \forall \omega \tag{D.13}$$

where expression (D.11) will replace $\tilde{u} \cdot \tilde{h}$ in the objective function, and equations (D.12)-(D.13) should be part of the set of constraints.

Appendix E. Algorithms for Solving MINLP and NLPP.

NLPP problem is solved by decomposition. A Lagrangian relaxation is applied to **NLPP** to decompose the problem by ω. (E.1) shows the Lagrangian relaxation expression, where $\mu = (\mu_o; o \in O)$ is the vector of Lagrange multipliers for the relaxed constraints $g_2 \leq 0$ in (30a) (that is, (17) evaluated at $\mathbf{y}^{(s)}$ and, for simplicity, $D_o^{(s}$ represents its right hand side.

$$\mathcal{L}(\mathbf{x}, \mathbf{y}^{(s}, \mu) := \ F(\mathbf{x}) + \sum_{o \in \mathcal{O}} \mu_o \left(D_o^{(s} - \sum_{\omega \in W} \sum_{r \in R(\omega,o)} U_r^{\omega} h_r^{\omega} \right) \tag{E.1}$$

The new term in (E.1), added to $F(\mathbf{x})$ (the **NLPP** objective function), can be expressed as a sum of terms depending on ω plus a term depending only on μ variables.

The Dantzig Cutting-Plane algorithm decomposes the original problem **NLPP** into one non-linear primal subproblem, the Lagrangian relaxation of **NLPP** as appears below in $\mathcal{L}$-**NLPP** (E.2), and one linear master problem, **DZLP** (E.3). Let $(k$ be the iteration number for the Dantzig Cutting-Plane algorithm. Note that $(s$ is the iteration number drawn from algorithm 1, which reflects the fixed value for $\mathbf{y}$ variables. The Dual-Lagrangian function ϕ, corresponding to the lagrangian (E.1), for a point $\mathbf{y}^{(s}$ evaluated at $\mu^{(k}$, $\phi(\mu^{(k}, \mathbf{y}^{(s)})$, is evaluated at each non-linear primal subproblem $\mathcal{L}$-**NLPP**. It is given by:

$$(\mathcal{L}\textbf{-NLPP}) \quad \phi(\mu^{(k}, \mathbf{y}^{(s)}) \triangleq \min_{\mathbf{x}\in X} \mathcal{L}(\mathbf{x}, \mathbf{y}^{(\mathbf{s}}, \mu^{(k}) := \tag{E.2}$$

$$\min_{\mathbf{x}\in X} F(\mathbf{x}) - \sum_{\omega\in W} \sum_{o\in\mathcal{O}} \sum_{r\in R(\omega,o)} (\mu_o^{(k} U_r^\omega) h_r^\omega + \sum_{o\in\mathcal{O}} \mu_o^{(k} D_o^{(s}$$

$$\text{s.t. (30a)}$$

and the master problem is defined by:

$$(\textbf{DZLP}) \quad \max_{z,\mu} \; z \tag{E.3}$$

$$z \le F(\mathbf{x}^{(k)}) + \sum_{o\in\mathcal{O}} \mu_o \left(D_o^{(s} - \sum_{\omega} \sum_{r\in R(\omega,o)} U_r^\omega h_r^{\omega(k} \right) \Bigg| \; \alpha_k \quad , \forall k$$

$$z, \mu \in \mathbb{R}, \; \mu \ge 0$$

where α_k are the non-negative dual variables associated to the constraints.

The problem $\mathcal{L}$-**NLPP** can be decomposed into ω-subproblems. Let $\mathbf{x}_\omega$ be the subset of variables $\mathbf{x}$ that corresponds to ω, $\forall \omega \in W$. Subproblem $\mathcal{L}$-**NLPP**-ω (E.4) corresponds to each ω-decomposition of $\mathcal{L}$-**NLPP**.

$$(\mathcal{L}\textbf{-NLPP-}\omega) \quad \min_{\mathbf{x}_\omega} \mathcal{L}_\omega(\mathbf{x}_\omega, \mathbf{y}^{(s}, \mu^{(k)}) := \tag{E.4}$$

$$\min_{\mathbf{x}_\omega} F(\mathbf{x}_\omega) - \sum_{o\in\mathcal{O}} \sum_{r\in R(\omega,o)} (\mu_o^{(k} U_r^\omega) h_r^\omega$$

$$\text{s.t. subset of (30a) that corresponds to } \omega$$

After solving $\mathcal{L}$-**NLPP**, a feasible solution can be obtained from the dual variables α_k of the last master problem **DZLP** solved: $\mathbf{x}^* = \sum_k \alpha_k \mathbf{x}^{(k}$. Moreover, the Dantzig Cutting-Plane's algorithm requires an initial feasible solution: in this case, a good option is to take advantage that the solution of the problem **MLMP** is feasible for the problem **NLPP**.

The algorithm for solving **MINLP** is shown in Algorithm 1. Also, the application of the Dantzig Cutting-Plane's algorithm for solving problem **NLPP** results in the following Algorithm 2.

Algorithm 1: Solving MINLP

initialization
- Find a feasible point $\hat{\mathbf{x}}, \mathbf{y}^{(0}$
- Let $s = 0$
- Fix ϵ

while *not STOP* **do**
- Solve $\mathbf{NLPP}(\mathbf{y}^{(s)})$, with $\hat{\mathbf{x}}$ as initial solution: $\rightarrow \mathbf{x}^{(s}$
- UBD $= F(\mathbf{x}^{(s)})$
- Solve **MLMP** $\rightarrow z^*, \mathbf{x}^*, \mathbf{y}^*$
- **if MLMP** *has no feasible solution* **then** STOP
- **else**
  - LBD $= z^*$
  - **if** *(UBD-LBD)/LBD* $< \epsilon$ **then** STOP
  - **else**
    - $s + 1 \rightarrow s$
    - $\mathbf{y}^* \rightarrow \mathbf{y}^{(s}$
    - $\mathbf{x}^* \rightarrow \hat{\mathbf{x}}$

return $\mathbf{x}^{(s}, \mathbf{y}^{(s}, F(\mathbf{x}^{(s)})$

Algorithm 2: Solving $\mathbf{NLPP}(\mathbf{y}^{(s)})$

Input: $\mathbf{y}^{(s}, \hat{\mathbf{x}}$

Output: $\mathbf{x}^*, F(\mathbf{x}^*)$

initialization
- $\hat{\mathbf{x}} \rightarrow$ **NLPP** initial feasible point $\mathbf{x}^{(0}$
- Let $k = 1$
- Fix $\hat{\epsilon}$

while *not STOP* **do**
- Solve **DZLP** $(\mathbf{x}^{(k-1)})$: $z^\star, \mu^\star \rightarrow z^{(k}, \mu^{(k}$ dual variables of **DZLP** $\rightarrow \alpha_i$, $i = 1, \ldots, k$
- Solve $\mathcal{L}$-**NLPP** by decomposition in $\mathcal{L}$-**NLPP**-ω subproblems
- $\mathbf{x}^\star_\omega, \ \forall \omega \rightarrow x^\star \rightarrow x^{(k}$
- $\mathcal{L}_\omega(\mathbf{x}^\star_\omega, \mathbf{y}^{(s}, \mu^{(k)}), \ \forall \omega \rightarrow \mathcal{L}(\mathbf{x}^\star, \mathbf{y}^{(s}, \mu^{(k)})$
- **if** $(z^\star - \mathcal{L}(\mathbf{x}^\star))/\mathcal{L}(\mathbf{x}^\star) < \hat{\epsilon}$ **then** STOP
- **else** $k + 1 \rightarrow k$

NLPP-feasible solution
- $\mathbf{x}^* = \sum_{i=1}^{k} \alpha_i \mathbf{x}^{(i}$
- Calculate $F(\mathbf{x}^*)$

return $\mathbf{x}^\star, F(\mathbf{x}^\star)$

Appendix F. Data sources.

Utility criteria. The first step is to define the explanatory variables for the systematic term of the generalized cost functions (22). The criteria for choosing them must rely on their usage in common data surveys and be easy to calculate for the corresponding transportation mode. Four variables were chosen: distance, travel time, price, GHG-emissions. Also, a dummy variable for each type of product transported was added: A 0-1 value, to try to catch special characteristics for each product when transported.

- **Distance**. Information was obtained from Ecotransit (Ifeu et al. (2016)), a web tool for calculating transportation environmental impacts.
- **Travel time**. For train, data is calculated from TPNOVA (2020), a rail operator agency's web page with calculator for train freight transportation. For road, a calculation was applied based on the average speed for trucks for international freight transport and taking into account mandatory time to rest during the trip.
- **Price**. For train, again TPNOVA gives an approximation, complemented with information from other sources, as DB Cargo AG (2019), Martínez et al. (2015) or Pérez (2015). For road, the data used is the average price per kilometer for international transport by road calculated from work presented in Martínez et al. (2015), Pérez (2015), and taking into account that prices of road transport remained steady since 2014 (Secretaría General de Transporte (2020)).
- **GHG-emissions**. Data obtained from Ecotransit (Ifeu et al. (2016)). It was parameterized for transporting two TEUs of 10 t/TEU, from origin yard to destination yard, for both truck and train, using the standard parameters:

  Truck: a diesel vehicle of 26-40 t, with a load factor of 95.77% and empty trip factor of 20%.

  Train: an electrified container train of 1000 t, with a load factor of 49.8% and empty trip factor (ETF) of: 20%
- **A dummy variable for each product**. A 0-1 value, to try to catch special characteristics for each product when transported.

Selection of product type and OD-pairs. From Datacomex (Datacomex (2020)), the statistics' web for Spanish Foreign trade, the criteria was to select origin and destination pairs and the products transported between them, which had rail as one of their modes of transport during last years (2015-2018), and with origin or destination in Catalunya, Comunidad Valenciana or Aragón. The countries selected were France, Germany, Italy, the Netherlands, Belgium, and Poland. Products selected were Vehicles, Fruits and vegetables, Chemical products, Automotive complements, Grain, and Steel and Iron.

Calculation of additional parameters. Different works about costs on rail freight transportation (Guinot (2008), Institut Cerdà (2019)), jointly with public information from infrastructure managers about prices for their services (ADIF (2020),DB Cargo AG (2019), SNCF Réseau (2020), Deutsche Bahn AG (2020)) are the basis to estimate the cost for rail freight transport.

Infrastructure and definition of rail corridors. Infrastructure characteristics are defined from public data offered by infrastructure managers (ADIF (2020), SNCF Réseau (2020), Deutsche Bahn AG (2020)). Examples tests are based on five carriers, and the definition of their rail corridors, connections and frequency is based on public information about rail freight corridors in Europe.

Appendix G. Parameters of utility function estimation.

Table G.6: Disutility function parameters for the tests

utility component		mode	unit	Estimate	confidence interval		β^-	β^+	
					2.5%	97.5%			
β_0	(Intercept)	train	-	4.6549	4.3410	4.9688	4.6549	0.3139	
$\tilde{\beta}_d$	distance	truck	km	0.0051	0.0036	0.0065	0.0051	0.0015	$\star$
β_d	distance	train	km	0.0051	0.0036	0.0065	0.0051	0.0015	$\star$
$\tilde{\beta}_{co}$	GHG-emissions	truck	kg	0.0006	0.0006	0.0007	0.0006	0.0001	$\star$
β_{co}	GHG-emissions	train	kg	0.0006	0.0006	0.0007	0.0006	0.0001	
β_p	price diference	train	€	0.0009	0.0003	0.0015	0.0009	0.0006	$\star$
β_{ac}	automot.compl	train	0/1	-0.5919	-1.0091	-0.1747	-0.5919	0.4172	$\star$
β_{gr}	grain	train	0/1	-0.8612	-1.8832	0.1608	-0.9416	0.9416	$\star$
β_{fv}	fruits& veget	train	0/1	1.3259	0.9342	1.7176	1.3259	0.3917	$\star$
β_{ch}	chemical prod	train	0/1	-0.3365	-0.5487	-0.1244	-0.3365	0.2121	$\star$
β_{ve}	vehicles	train	0/1	-4.7270	-4.9468	-4.5072	-4.7270	0.2198	
β_{OD}	OD decrease	train	0/1	-2.0661	-2.2039	-1.9283	-2.0661	0.1378	
β_{od}	OD increase	train	0/1	2.9888	2.6566	3.3209	2.9888	0.3321	

McFadden R^2: 0.37632

As it is said, a logit approximation was applied to estimate the values for β-parameters. The first difficulty was related with the linear dependency among the explanatory variables, especially between **GHG-emissions** with **distance** and **price**, for train data, and **distance** with **travel time** and **price**, for road data. Different combinations of the variables were tested, with no satisfactory results:

either some parameter was not significant or had the wrong sign, or the adjustment was poor. A combination of **distance**, **GHG-emissions** and a new variable defined as the train price minus road price (named as **price difference**), jointly with the dummy variables per product, seemed to fit the data. Nevertheless, new adjustments were necessary: first, the **price difference** were not appropriated for some products, as vehicle or chemical products. In these cases, **price difference** was not applied. Also, because of the special characteristics of train transport, a few combinations of OD-pairs and product have very different behavior in terms of train share. For these particular OD-pairs-product combinations, two new dummy variables were defined: one, named **OD decrease**, which helps to reduce train costs (and to increase train share); other, named **OD increase**, which helps to raise train costs (and to diminish train share).

The results after calibration can be seen in Table G.6, which shows the mean estimate, the limits for the 95%-confidence interval and the values for β^-, β^+ parameters. All of the β^-, β^+ parameters were calculated from the confidence interval. The symbol $*$ marks those parameters to which the robustness criteria is applied. The dummy variable for steel & iron products was the reference variable. Also, the road was the reference mode. All parameters are correct in sign, and all have a good level of significance. Some products are more suitable to transport by train than others, as the difference (both in sign and value) among the dummy variables for product shows. A value of 0.38 for the R^2 of McFadden shows a good adjustment for the model.