Graph neural network-guided optimization for intermodal transport planning under uncertainty

Javier Durán-Micco*[1], Bilge Atasoy[1]

[1] Maritime and Transport Technology, Delft University of Technology, The Netherlands

SHORT SUMMARY

This paper addresses the Service Network Design (SND) problem faced by a Logistics Service Provider (LSP), integrating tactical planning with dynamic operational decisions. The proposed approach considers a complex operational setting, including uncertain travel times and demand, dynamic replanning decisions, and interactions between the LSP and carriers. An agent-based simulation model is developed to capture these complexities and is coupled with a metaheuristic to solve the SND. To overcome the high computational cost of simulation, a Graph Neural Network (GNN) is introduced as a surrogate model. The GNN, trained with simulation-generated data, leverages the network structure to predict both global performance (profit) and node-level indicators, which are used to guide the search process. Numerical experiments show that the proposed framework produces high-quality solutions with scalable computational effort, particularly for large-scale instances. The results highlight the potential of integrating optimization and machine learning to address complex freight transport planning.

Keywords: Freight transport planning, service network design, graph neural network, metaheuristics, agent-based simulation.

1. INTRODUCTION

Logistics Service Providers (LSPs) play a central role in coordinating complex freight transport systems, by consolidating shipments and orchestrating transport across multiple modes and carriers. This coordination, however, leads to complex planning problems involving multiple decision levels and significant sources of uncertainty. A key tactical problem faced by LSPs is the Service Network Design (SND) problem, which determines service selection and capacity allocation to satisfy transport demand. While classical SND formulations are typically deterministic, real-world freight systems are subject to substantial uncertainty, particularly in travel times and demand. These challenges are amplified in multimodal settings, where coordination between flexible road transport and scheduled services (e.g., rail and inland waterways) is required (Crainic & Rei, 2025).

Recent research has incorporated stochastic elements into SND through approaches such as scenario-based stochastic programming, robust optimization, and simulation-based methods. However, important limitations remain. Many studies focus on unimodal systems or simplified multimodal settings, and most rely on two-stages optimization over predefined scenarios, limiting their ability to capture dynamic and adaptive decision-making (Crainic & Rei, 2025; Delbart et al., 2021). Simulation offers greater flexibility to represent uncertainty and operational dynamics in detail. However, its high computational cost has limited its integration within optimization frameworks for the SND (Hrušovský et al., 2018; Layeb et al., 2018).

To address these challenges, this paper proposes a hybrid solution framework for a stochastic, multimodal SND problem that explicitly integrates tactical planning with dynamic operational decisions. The approach combines a metaheuristic algorithm to solve the tactical problem, with an agent-based simulation model that represents the daily operations. The proposed framework builds on previous work, where a metaheuristic aided by a regression model was proposed to address a simpler version of the problem (Durán-Micco & Atasoy, 2026). In this paper, the problem context is extended to capture also stochastic demand in addition to uncertain travel times, and the simulation is enhanced with adaptive interactions between a LSP and carriers. To overcome the high computational cost of simulation-based evaluation and efficiently address the added problem complexity, we incorporate a Graph Neural Network (GNN) as a surrogate model. By exploiting the underlying network structure, the GNN learns to approximate both global performance metrics and node-level indicators, enabling not only the prediction of the total profits of a candidate solution, but also providing information to guide the search toward better solutions.

The proposed framework enables the efficient solution of large-scale stochastic SND instances, providing high-quality solutions while maintaining tractable computational times. The results highlight the potential of combining simulation-based optimization with learning-based surrogates for complex transport planning problems.

2. PROBLEM DESCRIPTION

This paper considers a complex variant of SND that includes multiple transport modes, scheduled services, uncertain travel times and demand, and dynamic interactions among actors (LSP, carriers, and shippers) with recourse actions to react to uncertainty. As shown in Figure 1, the problem is formulated as a bilevel structure: tactical decisions by the LSP at the upper level, and dynamic operational decisions by all actors at the lower level. Tactical decisions are made once and define the operational scenarios over a representative planning horizon (e.g., one week).

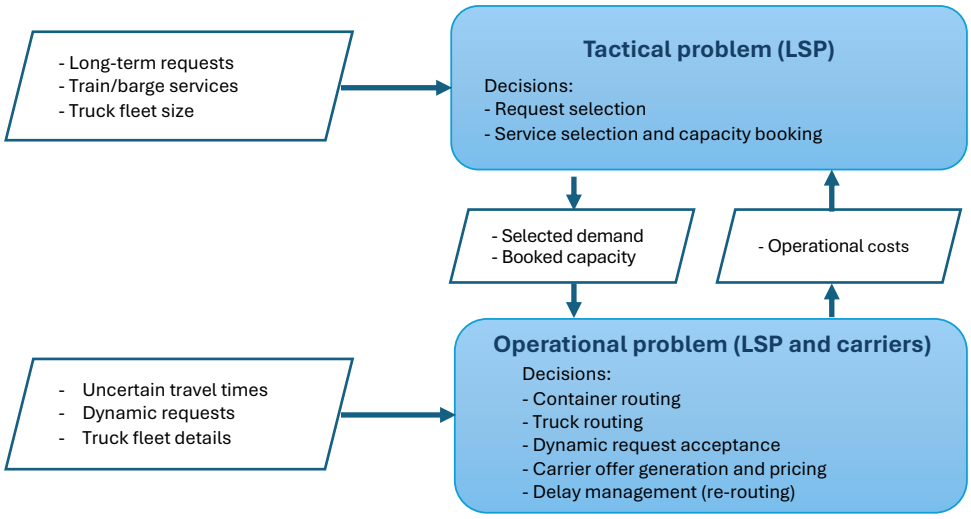


Figure 1: Schematic representation of SND as bilevel problem.

We consider a multimodal transport network represented by a graph $G(N, A)$, with three transport modes: road, rail, and inland waterways (IWW). Nodes N represent intermodal terminals, customers, and truck depots. Arcs A capture modal connections: road links connect all nodes, while

rail and IWW connect selected terminals. Truck operations differ from rail and IWW. A limited fleet of trucks, managed by one or more carriers and distributed across depots, operates flexibly within the network. In contrast, rail and IWW rely on predefined scheduled services composed of service legs, each defined by origin, destination, capacity (in containers), price, and fixed departure/arrival times. Finally, demand consists of transport requests (long-term and dynamic) characterized by origin, destination, volume (in containers), reward, and time windows.

At the tactical level, the LSP decides how much capacity to book on each scheduled service leg and which long-term requests to accept. At the operational level, the LSP executes transport using the booked capacity in scheduled services, contracted carrier trucks, or external trucks (assumed always available at a higher cost). In addition to planned demand, stochastic dynamic requests may be placed by shippers and be accepted or rejected by the LSP. Carriers offer truck services to the LSP, setting prices and routing their fleets accordingly. The LSP's objective is to maximize expected profit. Revenues from long-term requests and costs of booking of slots in scheduled services are deterministic, while revenues from dynamic requests and costs for trucking, storage, transfers, and delay penalties are stochastic. At the operational level, carriers also maximize their own profit, balancing service revenues against travel costs and delay penalties.

Uncertainty arises from both demand and road travel times. Each road arc has a travel time distribution, realized for each truck movement during execution. This may cause delays and missed connections with scheduled services, triggering dynamic replanning by both LSP and carriers, including rerouting of containers and trucks. While simplified versions of the problem can be formulated as a two-stage stochastic program, we adopt a rolling-horizon framework with dynamic recourse and actor interactions. The operational level is therefore modeled using an agent-based discrete-event simulation, as detailed in the next section.

3. METHODOLOGY

Given the problem's complexity and the need to address medium- to large-scale instances, we propose a solution framework combining metaheuristics, simulation, and machine learning (see Figure 2). The metaheuristic explores the tactical decision space, while the evaluation of candidate solutions involves modelling the operational problem, for which a simulation model is implemented. However, to mitigate the high computational cost of simulation, we develop a GNN surrogate model. The GNN is trained offline on simulation-generated data and then used within the metaheuristic to efficiently approximate solution quality. Below, we briefly summarize the main components of the proposed approach. Further details on the metaheuristic and simulation model are provided in (Durán-Micco & Atasoy, 2026).

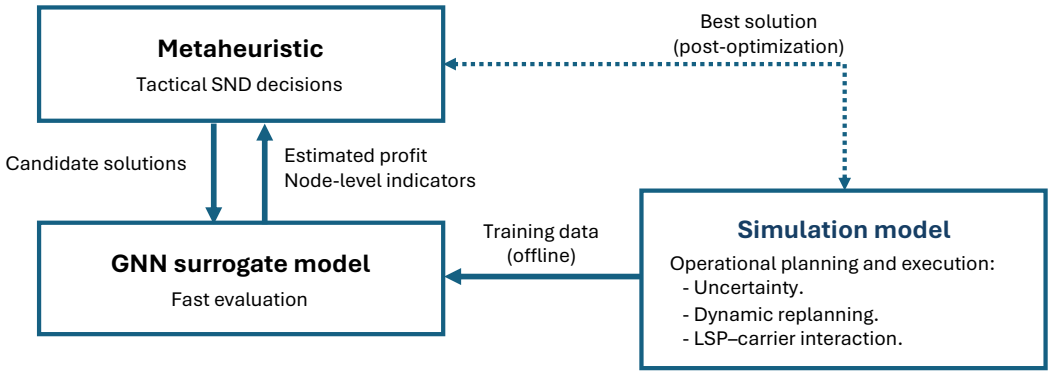


Figure 2: Integrated solution framework.

Simulation model

The operational level is modelled using an agent-based discrete-event simulation. Inputs include the physical network and the LSP's tactical decisions. The simulation tracks the movement of vehicles and containers, generates stochastic demand, realizes travel times, and triggers (re)planning decisions by the LSP and carriers. A schematic view of the simulation model is given in Figure 3.

The most relevant decision-triggering events are:

- **Start of the planning horizon:** The LSP determines routes for all containers associated with accepted long-term requests. Container-routing requires requesting quotes from carriers for individual truck legs. Carriers can make an offer, estimating marginal insertion costs and adding a profit margin.
- **Arrival of dynamic requests:** Upon receiving a stochastic request, the LSP evaluates feasibility, assigns a route, and makes an offer priced as expected cost plus a fixed margin. It is assumed that the shipper will accept the offer if this price is lower than the expected cost of external trucking.
- **Truck delays:** Travel times are realized upon arrival for each truck leg. Delays may cause missed connections for containers, both for the current load or for consecutive legs in the truck route. If that is the case, carriers first attempt to reassign affected containers within their fleet; if infeasible, they cancel the service (with compensation to the LSP), and the LSP has to replan the route for the affected containers.

The decision-making by the LSP and carriers are modelled by simple heuristics. The most relevant ones are:

- **Container routing (LSP):** When multiple requests must be routed, they are processed sequentially in arbitrary order. The routing involves deciding the sequence of legs to be followed, considering specific services and vehicles for each container. To generate the feasible paths, feasible combinations of scheduled services are precomputed, and combined with the truck legs (if necessary). For truck segments, the LSP requests quotes from carriers or uses an external provider, selecting the cheapest one. A feasible solution is always guaranteed (direct truck connection with external provider). The LSP finally chooses the cheapest feasible path(s), allowing splitting containers from the same request into different paths.
- **Container–truck allocation and truck routing (carriers):** This is handled through a sequential insertion heuristic that evaluates the best feasible insertion of each container into existing truck routes while respecting time window constraints. Routing decisions are integrated with the allocation process and must satisfy additional operational constraints, such as requiring each truck to return to its depot at the end of each working day.

The simulation runs over the full operational planning horizon. The primary output is the LSP's profit, along with auxiliary metrics such as accumulated delivery delays per node. This node-level indicator can be fed back into the metaheuristic to guide the search.

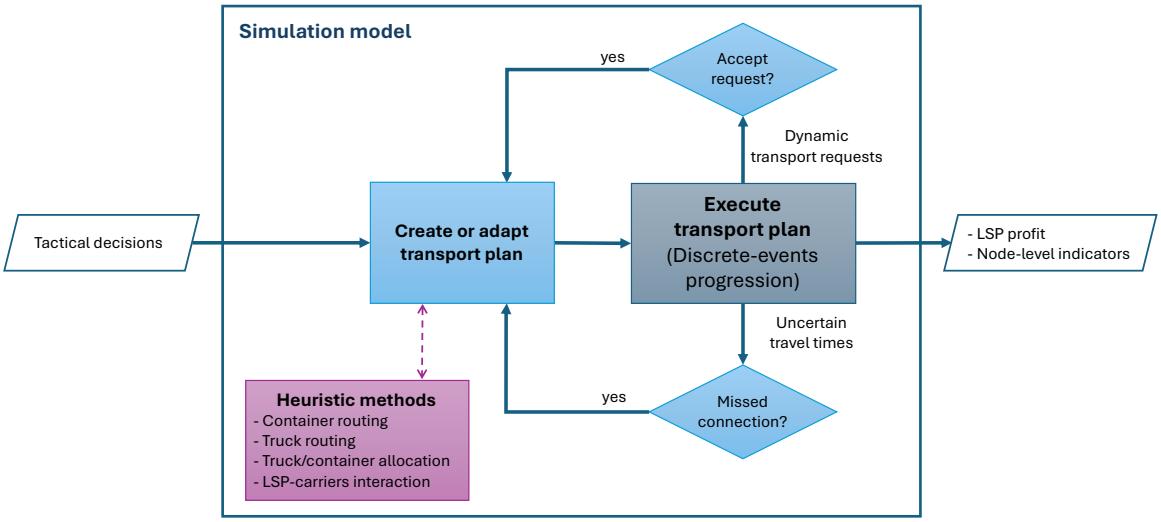


Figure 3: Schematic representation of the simulation model.

GNN

Simulation is computationally expensive, making it impractical to evaluate all candidate solutions as part of the metaheuristic algorithm. To address this, we develop a GNN surrogate model trained offline on simulation-generated data and used online to approximate solution quality.

The model follows a graph network architecture with joint node, edge, and global representations. The transport network is encoded as a graph with features capturing instance parameters, tactical decisions, and approximate container flows. The input features are defined at three levels:

- **Node-level:** incoming/outgoing demand, number of trucks at depots.
- **Edge-level:** services' capacity, long-term demand, distance by road, estimated flows.
- **Global-level:** aggregated demand, total booked capacity, and instance parameters.

Features are normalized and mapped to a latent space via linear encoders. The model then applies multiple message-passing layers with coupled updates: (1) edges are updated using incident nodes and global context, (2) nodes aggregate adjacent edge information and global features, and (3) the global state is updated using pooled node and edge embeddings. This allows information to propagate across the network while the model captures both local interactions and system-wide effects. Final predictions are obtained through separate heads: node-level accumulated delays and global expected profit. The model is trained in a supervised manner to replicate simulation outputs.

Metaheuristic

We propose an enhanced simulated annealing (SA) algorithm to solve the tactical SND problem. At this level, the decision variables are the selection of long-term requests and the capacity booked on each service leg. The SA uses a variable neighbourhood structure combining random and greedy operators. Random operators introduce perturbations in request selection and capacity levels. Greedy operators exploit feedback from the previous solution, specifically node-level delay information. The node with the highest accumulated delay is identified, and targeted modifications are applied to reduce congestion, either by decreasing selected demand destined for that node or by increasing capacity on services serving it. At each iteration, operators are selected probabilistically according to predefined weights. Candidate solutions are evaluated using either

the simulation model or the GNN surrogate, both providing estimates of total profit and node-level delays. The algorithm runs for a fixed number of iterations and returns the best solution found.

4. RESULTS AND DISCUSSION

This section presents numerical experiments evaluating the proposed framework. A previous version of the SA was benchmarked in (Durán-Micco & Atasoy, 2026), showing strong performance against exact methods for small deterministic instances and state-of-the-art metaheuristics for larger ones. A linear regression surrogate was also tested under stochastic travel times, leading to competitive results. Here, we extend the analysis to address a more complex stochastic setting with uncertainty in both demand and travel times, and explicit interactions between LSPs and carriers.

The SA and simulation model are implemented in C++, while the GNN is developed in PyTorch. The GNN consists of 3 message-passing layers with a hidden dimension of 16 (7714 parameters). It is trained on a dataset of solutions evaluated via simulation, covering a wide range of solution qualities and instance parameters (e.g., travel time variability, fleet size, demand levels). The dataset is divided into training (22680 samples), validation (4860), and test (4860) sets. A weighted loss (70% global, 30% node-level) is used for training. Data generation requires 0.68 h and training 0.31 h. On the test set, the model achieves an R^2 of 96.7% (MAE: 18.8) for profit prediction and 84.4% (MAE: 202.0) for node-level delays.

Experiments are conducted on a network based on the hinterland of the ports of Antwerp and Rotterdam (Figure 4), including 17 terminals, 46 customer locations, and 11 truck depots. The network includes 32 rail and 68 IWW services over a planning horizon of 280 hours. Road connections exist between all nodes, with travel times ranging from 90% to 120% of nominal values (beta-distributed). Instances vary by the number of long-term requests (50, 100, 200, 400, and 1000), with dynamic demand and fleet size scaled accordingly.

Due to the lack of benchmark results in the problem, we test the performance of the methods by comparing three variants of SA, differing in the solution evaluation mechanism: linear regression (SA_{reg}), GNN (SA_{gnn}), and simulation (SA_{sim}). Since the regression model predicts only profit, greedy operators are not used in SA_{reg}. Each experiment includes 10 SA runs, and in each case, the best solution found is finally evaluated via simulation.

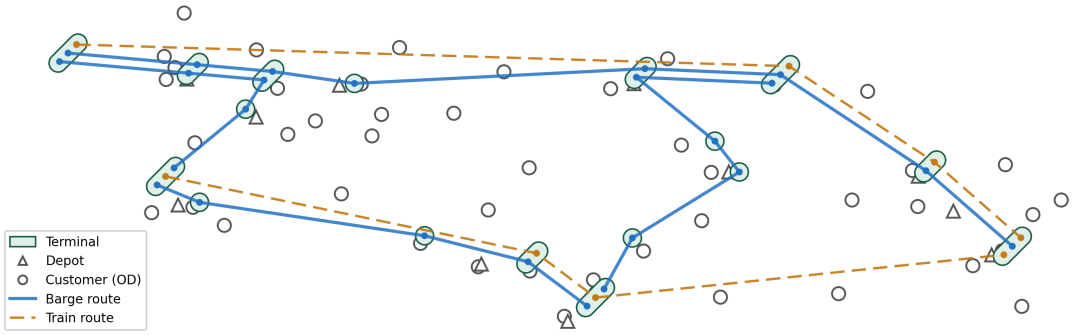


Figure 4: Network structure of the test instances.

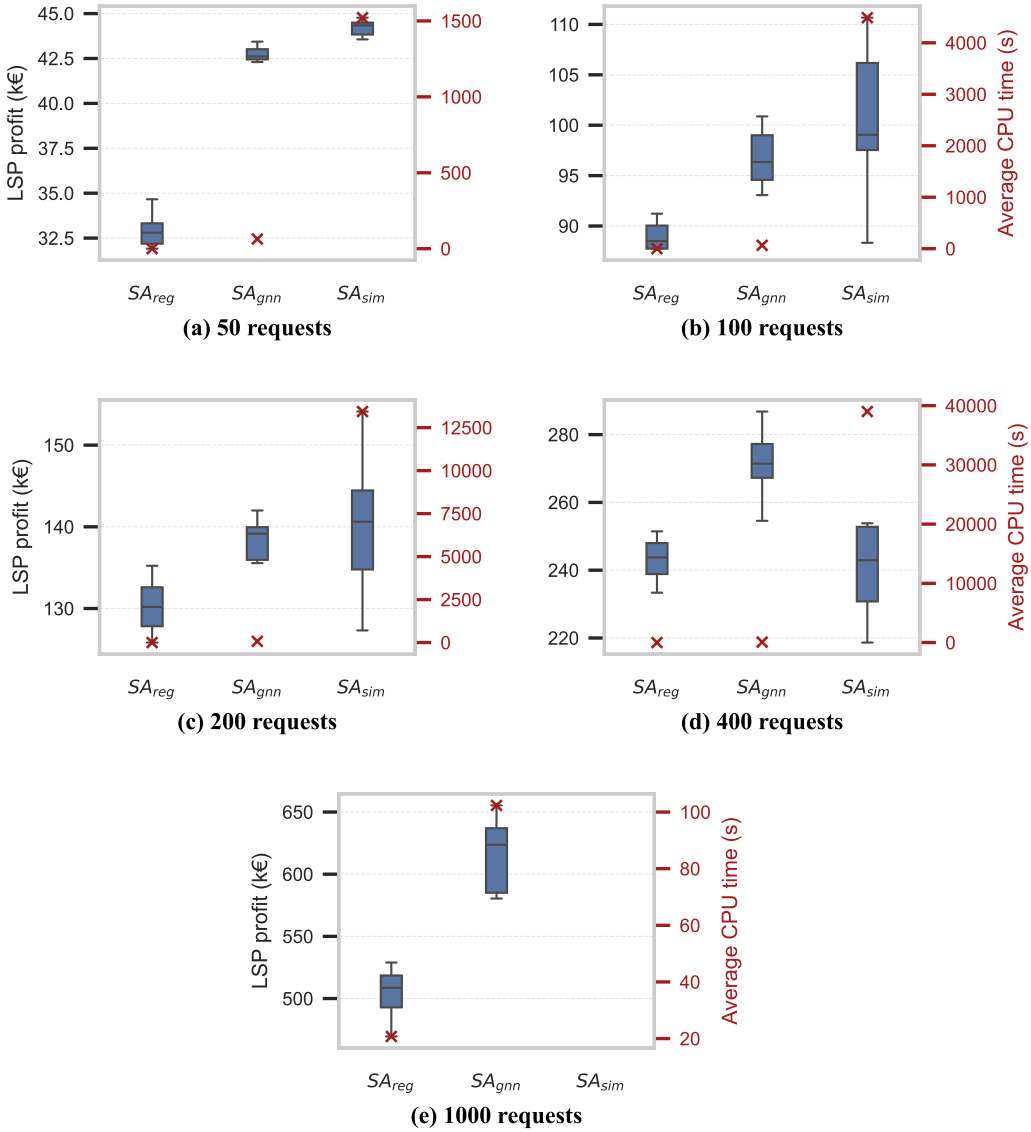


Figure 5: Comparison of algorithm performance: best solution values (boxplots) and average CPU time (markers) across SA replications.

The results in Figure 5 show that SA_{sim} yields the best solutions for small instances, as expected. However, SA_{gnn} performs competitively and consistently outperforms SA_{reg}. For larger instances (e.g., 400 requests), SA_{gnn} can even outperform SA_{sim} (by ~10%), likely due to the implicit noise in GNN predictions promoting search diversification, necessary in more complex instances. For the largest instance (1000 requests), SA_{gnn} clearly outperforms SA_{reg} (by ~20%), while SA_{sim} is not executed due to prohibitive runtime. In terms of computation time, SA_{gnn} is significantly faster than SA_{sim} and scales better, while remaining more accurate than SA_{reg}. Even when accounting for dataset generation and training, the total computational effort is lower than a single SA_{sim} run on larger instances.

Overall, the results demonstrate that integrating the GNN with the metaheuristic allows to efficiently solve the stochastic SND problem, achieving high-quality solutions with substantially reduced computational cost. Although experiments are conducted on a fixed network, the graph-

based structure of the GNN suggests potential for generalization to other network configurations, which remains a direction for future work.

5. CONCLUSIONS

We propose a solution framework for a complex and realistic variant of the SND problem. The model is formulated as a bilevel system (tactical and operational levels), incorporating scheduled services, flexible road transport, uncertainty in travel times and demand, and dynamic re-planning with interactions between LSPs and carriers. The solution approach combines a metaheuristic algorithm with a GNN trained on simulation-generated data. The GNN not only estimates the objective value of candidate solutions, but also provides node-level predictions that are used to guide the search toward improved solutions.

The numerical experiments demonstrate the effectiveness of the proposed method, particularly for larger instances, where it produces high-quality solutions within limited computational time, compared to the baseline algorithms. These results highlight the potential of GNNs for complex transport planning problems. By leveraging network-level information during training and inference, GNNs can better capture system dynamics and provide predictions that effectively guide optimization, including both global objective estimates and node-level indicators. This structure also enhances the potential for generalization to solve instances with different network configurations.

Future work will investigate the sensitivity of performance to different GNN design choices and extend the analysis to alternative network topologies and parameter settings to further assess generalization. In addition, further research will focus on improving the integration between the GNN and the metaheuristic to enhance search efficiency and solution quality.

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REFERENCES

Crainic, T. G., & Rei, W. (2025). 50 years of Operations Research for the tactical planning of consolidation-based freight transportation. *EURO Journal on Transportation and Logistics*, *14*, 100157. https://doi.org/10.1016/j.ejtl.2025.100157

Delbart, T., Molenbruch, Y., Braekers, K., & Caris, A. (2021). Uncertainty in Intermodal and Synchromodal Transport: Review and Future Research Directions. *Sustainability*, *13*(7), Article 7. https://doi.org/10.3390/su13073980

Durán-Micco, J., & Atasoy, B. (2026, March 25). *Adaptive decision-making for stochastic service network design*. arXiv.Org. https://arxiv.org/abs/2603.24369v2

Hrušovský, M., Demir, E., Jammernegg, W., & Van Woensel, T. (2018). Hybrid simulation and optimization approach for green intermodal transportation problem with travel time uncertainty. *Flexible Services and Manufacturing Journal*, *30*(3), 486–516. https://doi.org/10.1007/s10696-016-9267-1

Layeb, S. B., Jaoua, A., Jbira, A., & Makhlouf, Y. (2018). A simulation-optimization approach for scheduling in stochastic freight transportation. *Computers & Industrial Engineering*, *126*, 99–110. https://doi.org/10.1016/j.cie.2018.09.021