Journal of Industrial and Systems Engineering
Vol. 17, Special issue: 20th Iranian International Industrial Engineering Conference
Autumn (October) 2025; pp. 126-137

An Optimization Model for Hazardous Material Car Positioning in Rail Shunting Yards to Minimize Derailment Risk and Shunting Operations

Mehdi Fallahi[1], Morteza Bagheri[12*], Mir Saman Pishvaee[1]
[1]*School of Industrial Engineering at Iran University of Science and Technology, Tehran, Iran*
[2]*School of Railway Engineering at Iran University of Science and Technology, Tehran, Iran*

Abstract
Rail transport of hazardous materials (Hazmat) carries significant risks, such as derailments leading to explosions, toxic spills, and environmental harm. This study presents an innovative integer programming model to optimize Hazmat car positioning in rail shunting yards. By incorporating position-specific derailment risks, operational constraints, and safety regulations, the model minimizes derailment hazards while enhancing efficiency. Utilizing the Max-Min Ant System algorithm, it reduces shunting operations by up to 14.1%, as validated through applying the proposed methodology on generated instances, all while ensuring safety compliance. This practical solution balances safety and operational performance, significantly improving the reliability of Hazmat rail transport. The approach paves the way for advancements in rail yard management and risk mitigation, offering a robust framework for safer and more efficient Hazmat handling.

Keywords: Car positioning; Shunting operations; Hazardous materials;

1. Introduction

In 2023, almost two million carloads of hazardous materials were transported across North America, underscoring the significant risks associated with rail transport of Hazmat[1]. These risks are amplified by historical incidents, such as the 2013 Lac-Mégantic disaster, which tragically killed 47 people, and the 1979 Mississauga derailment, involving propane and chlorine tankers, which led to the evacuation of over 200,000 people without fatalities[2]. Such events highlight the urgent need for strategies to reduce hazmat incident risks.

Current regulations, enforced by the Canadian Transport Commission and the U.S. Department of Transportation, mandate a minimum of five buffer cars between Hazmat cars and the locomotive, and at least one buffer car between incompatible Hazmat loads, aiming to reduce derailment risks. However, rooted in outdated practices, these rules struggle to accommodate modern operational complexities—such as variable train lengths and diverse derailment causes—limiting their efficacy[3, 4]. This limitation highlights the need for innovative, research-based solutions to improve safety in Hazmat rail transport.

Academic research has significantly advanced Hazmat risk management, evolving through distinct phases. Early studies focused on derailment patterns to determine optimal Hazmat car positioning. For instance, Fang and Reed [5] advocated positioning Hazmat cars at the train's rear, citing higher derailment risks at the front. Subsequent research by Nayak, Rosenfield and Hagopian [6] and Thompson, Zamejc and Ahlbeck [7] revealed that optimal positioning varies with derailment causes and train-specific factors, challenging the notion of a universal solution. The car positioning problem in railway transportation of hazardous materials involves determining the optimal positions for these cars within a train to minimize their risk of being involved in a derailment, taking into account the varying probabilities of different train sections being affected by such incidents.

---

[*] Corresponding Author ISSN: 1735-8272,

Building on these insights, probabilistic models emerged to provide a more precise assessment of derailment risks. Saccomanno and El-Hage [4] introduced a model demonstrating that derailment risk varies along a train's length, with strategic shunting reducing Hazmat involvement. Bagheri, Saccomanno and Fu [8] expanded this work with a risk-minimization framework, integrating operational conditions, track characteristics, and derailment causes. Their findings suggest that rear positioning is optimal for track-related derailments, while front positioning better mitigates risks from equipment failures, such as axle or wheel defects, offering a tailored safety approach.

Optimization frameworks further advanced the field, Verma [9] introduced a risk assessment framework that incorporates train length, the decile position of hazmat cars within the train, and the sequence of events leading to hazmat release. This framework enables the development of shunting strategies tailored to the specific risk profiles of different train routes and operational conditions, providing flexibility for operators to adapt to varying scenarios. Similarly, Bagheri, Saccomanno [10] proposed a hazmat car positioning framework that integrates in-transit risk models with rail yard shunting costs, emphasizing the need to balance the increased risk and time associated with shunting operations with the potential safety benefits of optimized car positioning. Their framework suggests that placing hazmat cars in positions least likely to derail—based on track attributes and route characteristics—is an effective strategy for reducing overall risk, highlighting the trade-off between operational efficiency and safety.

Advancing this further, Bagheri, Saccomanno and Fu [11] presented a Genetic Algorithm (GA)-based hazmat car positioning model that minimizes derailment risks while considering block integrity, ensuring that groups of cars remain intact during operations, which is crucial for maintaining operational flow. Rahbar and Bagheri [12] developed a Mixed-Integer Programming (MIP) model that incorporates rail yard constraints such as assembly time and operational costs, demonstrating that optimizing car positioning can significantly reduce derailment risks without excessive increases in operational complexity. Together, these studies highlight the power of optimization techniques to enhance safety within practical limits.

Cheng, Verma and Verter [13] study provides a foundational framework for understanding the interplay between train makeup and hazmat positioning, emphasizing the importance of nested assignment decisions and the research gap in commodity-based blocking. Their work suggests that integrating hazmat positioning into train assembly strategies can enhance safety, particularly in managing risks in transport corridors.

Considering Hazmat routing in railway network, Hosseini and Verma [14] utilized the VaR methodology to develop risk-averse routing strategies that account for low-probability, high-consequence events, providing a complementary approach to routing planning. Aiming resolving VAR measurement drawbacks, Hosseini and Verma [15] introduced a CVaR approach that emphasizes minimizing the risk of high-consequence derailments by considering worst-case scenarios and accounting for tail-end risks. Their model optimizes car positioning while factoring in train configurations, ensuring that hazmat cars are positioned to mitigate the most severe potential outcomes, which is a critical consideration for risk-averse operators. Hosseini and Verma [16] extended the application of the CVaR methodology to address the issue of risk equity, which refers to the fair distribution of hazmat risks across different segments of the rail network. While minimizing total risk is important, ensuring that certain population zones are not disproportionately exposed to high levels of risk is equally crucial. Their framework uses Lagrangian relaxation and subgradient optimization to solve this multi-commodity flow problem, balancing yard risk and arc risk to maintain risk equity across the network, offering a novel perspective on managing risk distribution in rail networks.

Operational analyses have also deepened our understanding of how train configuration affects derailment risks. Lin, Zhao [17] presented a probabilistic model assessing the likelihood and severity of derailments involving Hazmat cars, based on train configurations and accident characteristics, offering insights into trade-offs across unit and mixed freight operations. Lin, Liu [18]further quantified how derailment probability and severity relate to in-train car positioning, speed, and train composition, with a case study showing significant risk variations tied to these factors, though it lacked consequence modeling—an area needing further exploration.

Additional operational perspectives come from Kang, Zhao [19], who compared risks of transporting Class 3 flammable liquids in high-hazard flammable unit trains (HHFUTs) versus high-hazard flammable trains (HHFTs) with varied tank car positions. Their event-chain analysis identified positions 66–85 in HHFTs as the lowest-risk, operationally viable option, focusing on block-level optimization. Fang, Fu [20] developed a bi-level optimization model for routing multi-Hazmat railcars, integrating freight consolidation and a VaR approach to assess route risks. Their findings suggest that risk-seeking operators benefit from consolidation for cost savings, while risk-averse ones should increase train services, aligning strategies with decision-makers' risk preferences.

Most recently, [1] explored probabilistic modeling to optimize Hazmat car positioning, using a position-dependent, railcar-based method that considers train makeup, speed, length, and Hazmat car fraction. Their case study showed that optimal positioning shifts with operating conditions lower speeds favor rear positioning, higher speeds favor front distribution—reinforcing the absence of a one-size-fits-all solution and providing practical guidance for context-specific safety measures.

Despite significant research efforts, there is still no comprehensive model that simultaneously optimizes the positioning of Hazmat cars while incorporating risk assessment and needed shunting operations and operational constraints. Most prior studies have not developed a mathematical model specifically tailored to this challenge, nor have they offered a clear and practical methodology for quantifying shunting operations. One exception is the work by Rahbar and Bagheri [2], which does propose a mathematical model for Hazmat car positioning. However, their approach has notable limitations, particularly in how it handles shunting operation times. For instance, their model lacks clarity in defining the functionality of operations max time constraints and relies on a non-intelligent process for determining the of shunting operations. This inefficiency leads to an unnecessarily high number of operations across many cars.

In contrast, our proposed model takes a different and improved approach. It introduces a transparent and optimized method for quantifying shunting operations, addressing the shortcomings found in Rahbar and Bagheri's work. By better integrating operational constraints, our model provides a more practical and effective solution for positioning Hazmat cars, making it a significant advancement in this area.

This paper introduces an innovative optimization framework designed to bridge these gaps by incorporating risk assessment techniques alongside key operational considerations, such as yard constraints, assembly times, and economic factors. The primary objectives of this research are:

1. To develop an optimized model for hazmat car positioning in shunting yards,
2. To minimize derailment risks while maintaining operational efficiency, and
3. To validate the proposed model using real-world case studies.

By integrating these elements, this study offers a robust and practical approach to enhancing the safety and efficiency of railway operations involving Hazmat.

The remainder of this paper is organized as follows: Section 2 describes the problem context, Section 3 presents the proposed methodology, Section 4 illustrates a case study, and Section 5 discusses the results and concludes the paper.
The positioning of Hazmat railcars within shunting yards poses a critical operational challenge for railway systems. Effective positioning requires striking a delicate balance between minimizing derailment risks and optimizing train assembly efficiency. This complex optimization problem must fulfill stringent regulatory standards while addressing the inherent operational complexities unique to railway transportation systems.

2. Problem Description

Shunting yards serve a central role in organizing train compositions, acting as hubs where incoming railcars from diverse origins are systematically sorted, classified, and positioned within outbound trains. This sorting process is typically facilitated by dedicated yard engines that transfer cars from arrival tracks to specific classification tracks based on destination criteria. Among the most significant challenges in this process is ensuring that hazmat car positioning adheres strictly to regulatory compliance while simultaneously minimizing potential derailment risks, given that derailment probability for car positions varies significantly along the length of a train. Track-related defects, including broken rails, compromised roadbeds, or track misalignments, predominantly impact the front section of trains, while equipment-related failures, such as wheel or axle defects, generally affect cars situated toward the rear. Hence, achieving optimal hazmat car positioning requires comprehensive consideration of both the train’s operational parameters and the specific route characteristics it will encounter.

An essential consideration in optimizing hazmat car positioning is maintaining block integrity, which refers to the cohesive grouping of railcars that share a common destination. Although preserving block integrity significantly enhances operational efficiency, it frequently conflicts with safety objectives. For instance, positioning hazmat cars at the rear of a train can reduce exposure to derailment risks, but doing so may necessitate additional complex and time-consuming shunting operations, especially when hazmat cars within a block have different destination points. This inherent operational efficiency-safety trade-off mandates advanced and sophisticated planning to effectively optimize hazmat car positioning without sacrificing overall yard productivity.

The process of shunting itself introduces additional risk factors. Specifically, the activities involved in moving, coupling, and decoupling railcars inherently pose risks, which are further exacerbated when handling hazmat cars. Human error, miscommunication, or equipment malfunctions during the shunting process could potentially lead to Hazmat releases or serious incidents. Consequently, optimization strategies must carefully balance two competing forms of risk: the risks associated with hazmat car positioning during transit and the hazards arising from yard-based shunting operations. While reducing yard shunting maneuvers can mitigate yard-specific risks, this strategy may adversely affect the overall safety profile of the assembled train during its subsequent journey.

The fundamental tension between safety optimization and operational efficiency represents a core challenge for hazmat car positioning in shunting yard operations. Successful optimization requires achieving a derailment-resistant car arrangement, minimizing the frequency and complexity of shunting operations, and preserving block integrity.

Regulatory frameworks often compound these complexities by imposing positioning constraints that may conflict directly with optimal safety or operational efficiency objectives.

Contemporary optimization methodologies, including Genetic Algorithms (GA) and Mixed Integer Programming (MIP), strive to reconcile these competing goals. For example, Bagheri, Saccomanno [10] developed the Dangerous Goods (DG) positioning framework, which integrates rigorous transit risk assessments with detailed analyses of yard shunting costs. Their framework emphasizes that strategic positioning of hazmat cars in positions of minimal derailment probability, based on detailed evaluations of track and route characteristics, effectively lowers overall risk profiles. However, the associated benefits must be carefully weighed against the increased operational risks, resource demands, and time consumption resulting from intensified shunting activities.

This paper specifically addresses optimizing hazmat car positioning in a shunting yard characterized by multiple classification tracks, each dedicated to organizing blocks consisting of railcars headed toward shared destinations. These blocks typically include a heterogeneous mix of hazmat and non-hazmat cars. An additional track supports supplementary shunting operations without imposing any explicit capacity constraints, facilitating necessary rearrangements. Train assembly occurs on the departure track, where blocks are sequentially transferred following a predefined order. However, considerable optimization opportunities exist regarding car arrangements within individual blocks, given that block sizes vary but are predetermined and known.

The applicable regulatory framework categorizes Hazmat into clearly defined groups (A, B, C, D), as detailed in the General Operating Instructions of the Canadian Pacific Railway (Rahbar & Bagheri, 2014). Additionally, cars equipped with operational features such as ignition sources, mechanical heating devices, or cooling systems form a separate category (Group E). Non-hazardous cars constitute yet another group (Group F). The incompatibility matrix presented in Table 1 explicitly details positioning restrictions between these groups, marking prohibited adjacencies with '1' and permissible adjacencies with '0'.

Table 1 Incompatibility matrix between Hazmat type categories

		A	**B**	**C**	**D**	**E**	**F**
I=	A	0	**1**	**1**	0	**1**	0
	B	**1**	0	**1**	0	**1**	0
	C	**1**	**1**	0	0	**1**	0
	D	0	0	0	0	**1**	0
	E	**1**	**1**	**1**	**1**	0	0
	F	0	0	0	0	0	0

For analytical tractability and to limit computational complexity, the analysis assumes that only one car is moved per shunting operation. Although real-world scenarios frequently involve simultaneous multi-car movements, this simplification enables a focused examination of the core optimization challenge, providing a conservative upper bound on the required shunting operations.

While block sequencing in practical operations generally follows intermediate stop sequences, this research specifically targets optimizing hazmat car positioning to minimize derailment risks. Operational constraints that do not directly influence derailment risk are intentionally abstracted to clearly isolate and analyze the fundamental relationship between car positioning and derailment propensity.

The analysis incorporates several simplifying assumptions: the shunting yard remains isolated from external inbound or outbound trains during the shunting process, no railcars from external sources enter or leave during this period, and the analysis is confined to examining a single train formation event. These constraints are explicitly intended to simplify the scenario and allow for targeted exploration of the hazmat positioning optimization problem without introducing extraneous complexities from concurrent yard activities such as additional classification tasks, scheduling, or routing considerations.

3. Methodology

The suggested approach offers a detailed strategy for enhancing the arrangement of Hazmat cars in rail yard activities, tackling the intricate balance between reducing derailment risk of hazmat cars and ensuring operational efficiency. This approach integrates position-specific derailment probabilities, yard operational constraints, and regulatory requirements into a structured, multi-phase optimization process. By blending both predictable and unpredictable factors, the approach delivers a solid and practical solution for placing hazmat cars in real-world settings. It directly addresses the trade-offs between maximizing safety and maintaining operational flow, especially within yard shunting tasks and the preservation of train block structure. The strategy consists of three linked parts: (1) a risk evaluation system that calculates derailment chances based on a car’s position in the train, (2) a mixed integer programming model that arranges hazmat cars, minimizing risk of hazmat car derailment, and (3) a Max-Min Ant System algorithm that reduces the need for shunting movements. Together, these elements provide a thorough resolution to the hazmat car positioning challenge.

3.1. Framework Overview and Core Elements

The foundation of proposed methodological approach is grounded in an extensive analysis of accident data provided by the Federal Railroad Administration (FRA). This analysis has highlighted significant variations in derailment risks associated with car positions within train formations. Specifically, historical data indicates that railcars positioned at the front of trains are more vulnerable to track-related defects such as rail breaks, compromised track geometry, and roadbed deterioration. In contrast, railcars located toward the rear sections display a heightened susceptibility to equipment-related issues, notably bearing failures and wheel defects. Although real-world scenarios necessitate the calculation of position-specific derailment probabilities derived from historical data alongside track conditions, operational parameters, and equipment integrity, our current model leverages synthetic probability distributions. This approach effectively demonstrates the framework's practical capabilities and validates its underlying mathematical architecture.

The central optimization engine utilizes a sophisticated integer programming formulation designed to systematically allocate railcars to specific positions based on their derailment risk profiles. This mathematical model aims to minimize overall risk comprehensively while simultaneously ensuring operational practicality and adherence to regulatory standards. The formulation integrates deterministic constraints, reflecting mandatory regulatory requirements, with probabilistic components that account for the inherent uncertainty of derailment incidents. This dual-faceted approach allows the model to produce solutions that are practically feasible, fully aligned with the operational realities and constraints encountered in actual rail yard environments.

3.2. Structured Optimization Methodology

Proposed methodological framework suggests a structured five-phase approach (illustrated in Figure 1) designed specifically to manage the complexities involved in optimizing the positioning of Hazmat railcars. Each phase is constructed to address distinct aspects of the optimization challenge, balancing computational efficiency with practical application. The modular design of our framework allows each phase to be validated independently, ensuring comprehensive integration across the entire optimization procedure.

Phase 1: Generation of Block Permutations

This initial phase systematically generates all potential permutations of railcar blocks, with each block comprising a group of railcars headed toward a common destination. For a scenario involving n blocks, this generates n! potential sequences, laying the groundwork for subsequent optimization phases. The comprehensive enumeration ensures no

optimal arrangement is missed, facilitating structured and efficient computational implementation. As an example, three blocks labeled AA, KK, and CC yield permutations such as: (AA, KK, CC), (CC, KK, AA), (KK, AA, CC), (AA, CC, KK), (CC, AA, KK), and (KK, CC, AA).

Phase 2: Optimal Railcar Positioning

In this phase, an integer programming optimization model is formulated and solved for each generated permutation to determine optimal car positionings. This model incorporates:

- An objective function aiming to minimize overall derailment risk.
- Constraints to ensure block integrity, preserving operational coherence.
- Regulatory constraints governing required hazmat separation standards.

Phase 3: Solution Representation

Transformation Optimization results transition from detailed car-level assignments into a practical representation based on hazmat type classifications. This crucial transformation enhances practicality by treating railcars with the same hazmat type as interchangeable within their blocks. The simplified representation aligns with typical rail yard procedures, minimizing operational complexity and unnecessary shunting operations while maintaining safety.

Phase 4: Shunting Operations Calculation

A specialized adaptation of the Max-Min Ant System algorithm is employed, selected for its proven effectiveness in solving network-structured optimization problems. This algorithm applied on a network includes nodes (as a specific state of cars on in yard) and links (as transition of a state to another state). Each state represents the situation of all cars in the yard include the yard track and position in that track and the chain of moves from first state to that state is stored. The algorithm calculates an optimal sequence of single-car shunting movements required to transition from the current car arrangement to the optimized layout.

Although actual yard operations often involve simultaneous multi-car moves, the assumption of sequential single-car moves ensures computational feasibility and provides a clear basis for comparative analysis.

The operation calculation is structured based on a three-track system typical of rail yard infrastructure:

- Primary Track: Stores railcar blocks in their initial order and then during processing.
- Departure Track: Functions as the assembly point for the final train configuration, where blocks of cars are placed according to the optimized solution
- Auxiliary Track: Provides temporary storage to facilitate efficient shunting and reordering

This analysis begins with the *current state* of railcars, serving as the baseline for optimization. For illustration, consider three example blocks AA, KK, and CC, categorized by hazmat classification:

- Block AA: [A, B, F, F, F, … (25 cars)]
- Block KK: [A, B, C, F, F, … (33 cars)]
- Block CC: [A, B, B, C, D, F, … (59 cars)]

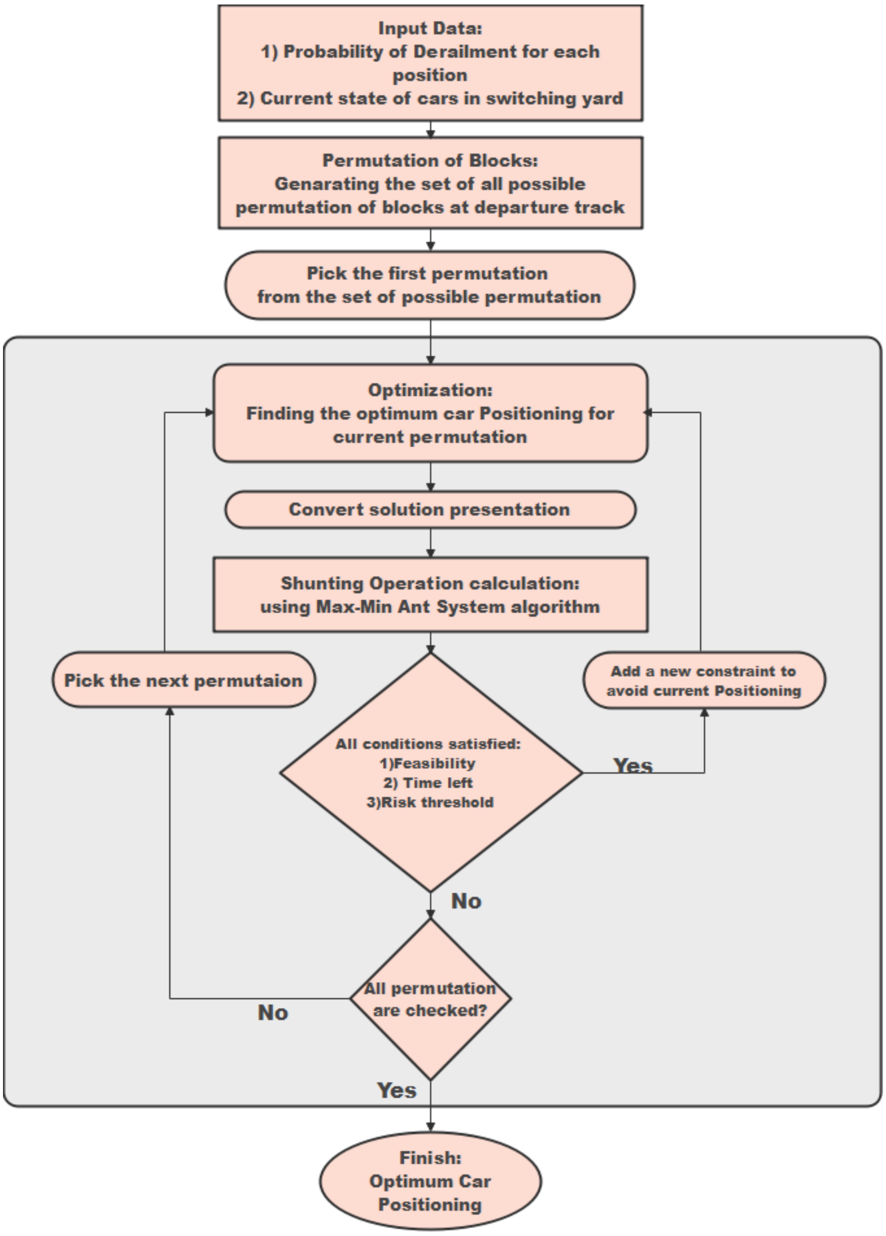

Figure 1 the proposed study framework

In this example, the first car in block AA is category A, the second is category B, with subsequent cars categorized as non-hazmat (F).

Phase 5: Iterative Optimization Refinement Following the initial analysis, this final phase implements an iterative refinement strategy to further enhance train configuration optimization while adhering to operational constraints. The refinement stage involves:

1. Dynamic constraint updates to prevent regeneration of suboptimal configurations.

2. Incorporation of constraints related to time limitations and acceptable thresholds for risk escalation, ensuring practical applicability and efficiency.

3.3. Extra Optimization Step

The optimization process employs an iterative improvement approach designed to systematically navigate the solution space, carefully balancing solution quality and computational efficiency. This approach comprises several essential components.

The refinement methodology for car positioning begins by evaluating initial arrangements against risk minimization objectives and operational constraints. It introduces additional constraints to steer the optimization toward enhanced configurations, ensuring continuous compliance with safety regulations. This process specifically focuses on identifying car positionings that maintain risk levels, reduce necessary shunting operations, uphold previous constraints as block integrity, comply with regulatory standards, and optimize the utilization of computational resources.

To enhance practical applicability, the optimization incorporates effective time management through a time-budgeted implementation. This strategy involves carefully allocating predefined maximum computation times to each permutation, adjusting dynamically based on the problem's scale. Specific termination criteria guide this time management, including reaching a predefined threshold of acceptable risk increase, exhaustion of the allotted time budget for extra optimization on shunting operations.

In the final optimization step, after assessing both risk values and required shunting operations across all permutations, an optimal permutation is chosen using a multi-criteria decision-making framework. The entropy-based weighted sum method, as outlined by Hwang & Yoon (1981) and Shannon (1948), was utilized to objectively integrate both criteria simultaneously. Unlike subjective methods, this entropy-based approach assigns objective weights derived from the intrinsic variation present in the data itself, eliminating biases inherent in subjective weighting. The method analyzes variations in each criterion across permutations, assigning greater weight to criteria exhibiting higher variability due to their increased informational content. Consequently, this ensures an objective balance between safety considerations (risk values) and operational efficiency (shunting operations). This method is particularly fitting for our optimization framework, as it systematically reduces potential biases when prioritizing between safety and operational efficiency, providing a robust and objective foundation for selecting the optimal solution.

3.4. Mathematical Model

The optimization model is formulated as an integer programming problem that considers safety objectives and practical constraints. The formulations are structured as follows:

Sets:

B	Set of blocks indexed by b
I_b	Set of cars in block b.
J	Set of positions in train indexed by j (1,..,TL).

Parameters:

P_j	Probability of derailment at position j
K	Required number of buffer cars between incompatible hazmat cars (=1).
I_{ab}	Incompatibility matrix element between hazmat categories a and b
TL	Total train length
SP_b	Starting position of block b in train
len(b)	Length of block b (number of cars)
F	Indicator for non-hazardous cars

Decision Variables:

x_{ijb}	Is 1 if car i in block b is placed at position j, 0 Otherwise.

Mathematical Model (for each permutation of blocks**):**

$$Min\ Z = \sum_{b\in B}\sum_{j=SP_b}^{SP_b+len(b)}\sum_{i\in b, i\neq' F'} x_{ijb} \times P_j \qquad \textbf{(1)}$$

$$\sum_{i\in b} x_{ijb} = 1 \qquad \forall\ b \in B,\ j \in \{SP_b,\ SP_b + len(b)\}, \qquad \textbf{(2)}$$

$$\sum_{j=SP_b}^{SP_b+len(b)} x_{ijb} = 1 \qquad \forall b \in B, i \in b \tag{3}$$

$$\sum_{j_1}^{TL-K+1} \sum_{j_2=\max(1,j_1-K+1)}^{\min(\mathrm{TL}+1,j_1+K)} x_{i_1,j_1,b_1} + x_{i_2,j_2,b_2} \leq 1 \quad \forall\, i_1 \in b_1, i_2 \in b_2\ , b_1, b_2 \in B, \\ I_{i_1,i_2} = 1, j_1 \neq j_2, if\ b_1 = b_2\ then\ i_1 < i_2 \tag{4}$$

The objective function (1) minimizes the overall derailment risk by strategically positioning hazardous cars within their designated blocks. The notation i≠F in equation (1) specifies that only hazardous cars are considered in the minimizing risk as objective function. In other word, the total risk is computed as the sum of derailment probabilities for each position (P_j) where a hazmat car is placed, weighted by position-specific risk values derived from historical data.

Non-hazardous cars (denoted as F) are excluded from the risk calculation, and the integrity of blocks is preserved according to defined position ranges SPb and len(b).

Constraint (2) ensures that every position j within block b is occupied by exactly one car from the same block, thereby maintaining the structural integrity of the train configuration.

Constraint (3) requires each car i within block b to be allocated precisely one position, thus preventing either repetition or omission of cars.

Constraint (4) enforces compliance with safety regulations by ensuring that hazardous cars classified as incompatible are not positioned within a specified range (K positions) of each other, guided by the incompatibility matrix I_{ab}. The incompatibility matrix is used to enforce constraints that prevent incompatible hazmat categories from being placed within one positions of each other, ensuring compliance with regulatory safety standards.

This formulation presents a mathematical framework that effectively integrates safety and operational considerations, maintains computational feasibility, supports practical implementation in real-world scenarios, and allows dynamic parameter adjustments based on yard conditions.

Having described the theoretical and mathematical foundations, the next section will validate this model through a practical case study, highlighting its applicability to real-world situations.

4. Case Study

To validate the proposed optimization model for Hazmat car positioning in shunting yards, the proposed algorithm was applied on some simulated instance problems considering simplified but realistic train formation scenarios. The purpose of this case study is to evaluate how effectively the model minimizes derailment risks while meeting operational constraints, including minimizing shunting operations. The experimental results highlight the computational efficiency and practical effectiveness of the methodology across various problem configurations. Important performance metrics assessed include risk reduction, improvements in operational efficiency, and computational demands.

4.1. Problem Setup

Six test instances were created to systematically assess the model's performance under diverse operational conditions. The primary parameters that varied across these instances included:

- Number of blocks per train: 3 and 5
- Sizes of each block: ranging from 10 to 70 cars
- Percentage of hazmat cars: 20%, 40% and 60% per block
- Total train length maintained at 120 cars

A representative test instance is provided below:
Block AA (15 cars): [A, B, F, F, F, ..., F]
Block KK (60 cars): [F, F, C, F, B, ..., F]
Block CC (35 cars): [B, B, F, C, D, F, ..., D]

Here, categories A-D indicate hazmat types, while F represents non-hazmat cars. The initial positions of cars within each block were randomized to evaluate the model's robustness in handling arbitrary initial positioning. To demonstrate the model's functionality, derailment probabilities (Pj) were randomly assigned to each car position, ranging between 0.005 and 0.05. Although these synthetic values are solely intended for validating the mathematical model and solution technique, actual derailment probabilities in real-world applications should be calculated based on historical data, considering track conditions, operational circumstances, and equipment characteristics. The complete methodology was implemented using Python, employing the CPLEX API to solve the integer programming model for each block permutation during the solution process.

4.2. Results

The experimental evaluation involves a thorough analysis of multiple problem instances, each with varying parameters. Detailed results are presented, focusing specifically on a representative instance to illustrate the algorithm’s performance. The optimization procedure incorporates position-specific derailment probabilities and aims to minimize repositioning operations, while respecting regulatory constraints for hazmat car arrangements.

Table 2 presents the comparative analysis of six distinct permutations for a problem with 3 blocks and 120 total car and 50% of Hazmat cars, evaluating both the objective function values and operational efficiency metrics. The objective function values exhibit notable consistency, ranging from 0.18082 to 0.18164. The total risk is calculated by adding up the derailment probabilities for each position where Hazmat cars are placed in the train. The permutation (BB, AA, CC) emerges as best solution, achieving operational efficiency with 152 shunting movements while maintaining an acceptable risk coefficient of 0.18082. The best permutation was selected using the entropy-based weighted sum method. This configuration demonstrated superior performance characteristics compared to alternative permutations, such as (CC, BB, AA), which exhibits both elevated risk (0.18164) and increased operational overhead (157 movements).

Table 2 objective function and number of shunting operations for each permutation

Permutation	Objective Value (Total risk)	BFS Number of Operations	Initial MMAS Number of Shunting Operations	Improved MMAS Number of Shunting Operations	Improvement
(AA, BB, CC)	0.18082	193	193	152	21.24%
(CC, AA, BB)	0.18089	175	175	149	14.86%
(CC, BB, AA)	0.18164	173	173	157	9.25%
(AA, CC, BB)	0.18089	153	153	145	5.23%
(BB, AA, CC)	0.18082	153	153	145	5.23%
(BB, CC, AA)	0.18164	147	147	139	5.44%

The improvements in the algorithm result in significant gains in operational efficiency. Quantitative analysis shows an average 12% reduction in shunting operations compared to the initial solution provided by the Min-Max Ant System (MMAS) algorithm, indicating the effectiveness of the improvement stage. Figure 2 shows the objective values include risk and the number of needed shunting operations for each possible permutation.

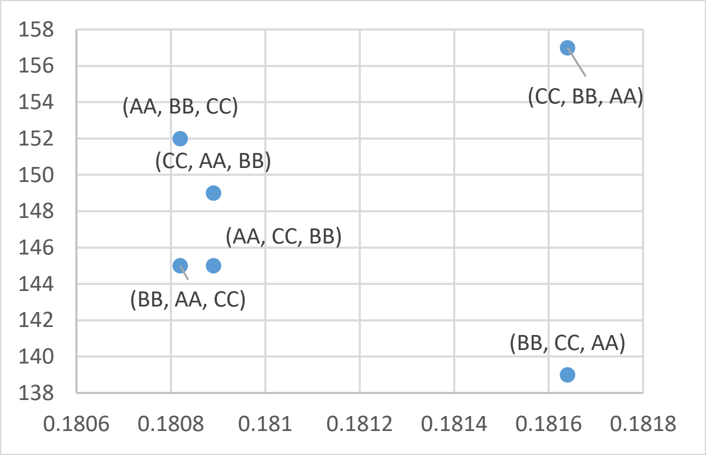

Figure 2 Improved MMAS number of shunting operations and risk Values for each permutation

Resolving the initial positioning problem consistently resulted in an average processing time of 0.15 seconds per permutation. A detailed computational performance analysis reveals varying temporal characteristics among different algorithmic methods. The Breadth-First Search (BFS) algorithm executed efficiently, with an average processing time of 0.03 seconds for minimizing shunting operations. The initial solution derived from MMAS demonstrated even greater computational efficiency, achieving near-instantaneous processing.

To validate the algorithm's effectiveness, a comparative analysis was performed against a BFS implementation. The analysis showed that our improved algorithm consistently provided superior operational efficiency, while ensuring feasibility and maintaining risk constraints established by the initial solution. This comparative advantage is particularly notable in terms of reduced shunting operations, a key performance indicator in practical railway operations.

Table 3 Computational results comparing across different problem configurations.

Problem	Train length (cars)	Number of Blocks	Hazmat Percentage	positioning time (sec)	(Total risk)	Initial MMAS Number of Shunting Operations	Initial MMAS Solution time (Sec)	Improved MMAS Number of Shunting Operations	Time budget for MMAS Improvement (sec)	Improvement in %
1	120	3	20%	0.15	0.1808	153	0.00	145	30	5.2%
2	120	5	20%	0.08	0.1906	155	0.05	142	30	8.4%
3	120	3	35%	0.19	0.5100	184	0.03	158	30	14.1%
4	120	5	35%	0.10	0.4785	178	0.09	154	30	13.5%
5	120	3	50%	0.16	0.9794	194	0.08	173	30	10.8%
6	120	5	50%	0.35	0.9503	205	0.03	178	30	13.2%

Computational results from six unique problem instances highlight the model's effectiveness and efficiency in optimizing the positioning of hazmat cars (Table 3). Each line is the best result for the given problem configuration (best permutation). Every instance maintained a uniform train length of 120 cars, but the number of blocks differed (3 or 5), and hazmat percentages varied (20%, 35%, or 50%). Notable patterns in the model's computational performance emerge, aligning with the complexity of the problem. Total risk values show a steady, monotonic rise as the hazmat percentage increases, ranging from 0.1808 to 0.9794, which confirms the model's risk assessment capabilities. In reducing shunting operations, the optimized Max-Min Ant System algorithm consistently surpassed both the initial MMAS and Breadth-First Search (BFS) approaches, with improvements spanning 5.2% to 14.1% than BFS number of shunting operations. The greatest improvement, 14.1%, occurred in the instance with 3 blocks and 35% hazmat content, while computational efficiency was upheld. Solution times for BFS steadily is near between 0.01 seconds, while the initial MMAS delivered consistently swift solutions in ≤0.01 seconds. All improvements were accomplished within a fixed 30-second time budget, illustrating the algorithm's ability to produce better solutions under practical computational limits. These findings affirm the model's success in balancing computational efficiency and solution quality across diverse problem configurations.

4.3. Discussion and Future Studies

This case study highlights several important findings. The Max-Min Ant System algorithm reliably reduced shunting operations by 5.2% to 14.1% compared to solutions provided by BFS algorithm, with the most notable enhancements occurring in scenarios containing 35% hazmat content. This improvement in operational efficiency, achieved by reducing the number of shunting operations while maintaining the same optimal objective value(risk), was accomplished without compromising safety. This demonstrates the model’s ability to effectively balance both operational demands and safety considerations. The model proved its versatility across hazmat levels ranging from 20% to 50%, underscoring its usefulness in a variety of operational contexts. That said, the growing computational demands observed at higher hazmat percentages point to possible scalability hurdles in highly complex setups.

Beyond computational gains, the reduction in shunting operations enhances safety by minimizing human error and equipment failure risks during yard activities, directly improving operational reliability and reducing exposure to yard-specific hazards.

The outcomes of this study open up several exciting possibilities for future investigation, grouped into three primary categories: methodological advancements, empirical testing, and operational improvements. On the methodological front, the existing model could be adapted to incorporate dynamic yard conditions, such as additional train arrivals during shunting or real-time shifts in track availability. Furthermore, adding real-time risk data—like weather conditions and track maintenance timelines—could refine the precision of derailment risk estimates. Testing the model on larger, more intricate rail networks would shed light on its scalability and resilience, especially under heavy traffic conditions. One vital research focus moving forward is determining position-specific derailment probabilities through empirical means. While this study relied on artificial probabilities to illustrate the model’s capabilities, future efforts should aim to compute real position-specific derailment probabilities using past derailment records. Such computations should factor in track features, train operating conditions, and equipment variables. Verifying the model with actual derailment probability distributions and accounting for distinct probability profiles between unit trains and manifest trains would markedly increase its real-world relevance. The model could also benefit from integrating block sequence restrictions tied to route planning and intermediate stops. This could be accomplished by factoring intermediate station operations into the overall shunting calculations or by assigning weights to block permutations based on their compatibility with the intended route. These refinements would more faithfully capture the practical challenges of manifest train service while continuing to prioritize hazmat risk reduction. Another valuable addition would be modeling multiple simultaneous car movements during shunting, aligning more closely with real yard practices and possibly revealing further efficiency gains. Implementing this would require tweaking the shunting analysis algorithm to manage the increased complexity of multiple car movements while keeping computations manageable. Successfully pursuing these research paths would significantly elevate both the theoretical framework of rail yard optimization and its practical deployment in operational settings. These upgrades would enhance the model's robustness and adaptability across diverse scenarios, all while preserving its central aim of minimizing hazmat transport risks.

4.4. Conclusion

This paper introduces an innovative optimization model designed for the positioning of hazmat cars in shunting yards, effectively harmonizing the goals of minimizing derailment risks and enhancing operational efficiency. The model's primary contributions encompass the incorporation of position-specific derailment risk assessments, the use of an incompatibility matrix tailored to various hazmat categories, and the enforcement of operational constraints through an integer programming approach. This cohesive methodology establishes a structured framework for optimizing the arrangement of hazmat cars while ensuring feasibility within yard operations.

Findings from the case study underscore the model's practical utility, revealing a reduction in shunting operations by as much as 14.1% without violating safety requirements. The model demonstrated its capability to optimize car positioning effectively across diverse scenarios, accommodating hazmat percentages ranging from 20% to 50% and varying block configurations, thus proving its robustness and versatility. A standout feature is its proficiency in delivering viable solutions that reconcile the typically opposing priorities of maximizing safety and sustaining operational efficiency.

An exploration of different block permutations exposed considerable disparities in derailment risks and the number of shunting operations needed, emphasizing the intricate nature of optimizing hazmat car positioning. The Max-Min Ant System algorithm emerged as highly effective, streamlining operational complexity while adhering to safety benchmarks, and it maintained computational efficiency even when applied to larger-scale problems.

The modular architecture of the optimization framework supports future enhancements without undermining its fundamental focus on risk reduction. Although this study employed synthetic derailment probabilities for illustrative purposes, the model is designed to seamlessly integrate real-world probability distributions, enhancing its relevance across a variety of operational settings and risk evaluation techniques.

This research markedly enriches both the theoretical insights into rail yard optimization and its actionable deployment. By delivering a thorough yet adaptable approach to hazmat car positioning optimization, the study propels advancements in rail safety management while preserving operational practicality. The model lays a robust groundwork for subsequent innovations in rail yard optimization, especially concerning the safe transport of Hazmat.

References

1. Lin, C.-Y., X. Liu, and C.P.L. Barkan, *Probabilistic modelling of optimal placement strategies of hazardous materials railcars in freight trains.* Accident Analysis & Prevention, 2025. **213**: p. 107957.
2. Rahbar, M. and M. Bagheri. *Formulation and Solution of a Risk Assessment Framework to Mitigate the Threat of Rail Transport of Hazardous Materials*. 2014. TRB 2014 Annual Meeting, http://amonline. trb. org/14-1592-1.2485122.
3. Bagheri, M., F.F. Saccomanno, and L. Fu, *Effective placement of dangerous goods cars in rail yard marshaling operation.* Canadian Journal of Civil Engineering, 2010. **37**(5): p. 753-762.
4. Saccomanno, F.F. and S.M. El-Hage, *Establishing derailment profiles by position for corridor shipments of dangerous goods.* Canadian journal of civil engineering, 1991. **18**(1): p. 67-75.
5. Fang, P. and H.D. Reed, *Strategic positioning of railroad cars to reduce their risk of derailment*, in *US DOT Volpe Transportation Systems Center (DOT/TSC), Cambridge, Mass*. 1979.
6. Nayak, P.R., D.B. Rosenfield, and J.H. Hagopian, *Event probabilities and impact zones for hazardous materials accidents on railroads.* 1983.
7. Thompson, R., E. Zamejc, and D. Ahlbeck, *Hazardous materials car placement in a train consist. Volume I, Review and analysis.* 1992.
8. Bagheri, M., F.F. Saccomanno, and L. Fu. *Risk-based model for marshaling dangerous goods railway cars in rail yards*. in *TRB 2009 - 88th Annual Meeting*. 2009.
9. Verma, M., *Railroad transportation of dangerous goods: A conditional exposure approach to minimize transport risk.* Transportation Research Part C: Emerging Technologies, 2011. **19**(5): p. 790-802.
10. Bagheri, M., et al., *Reducing the threat of in-transit derailments involving dangerous goods through effective placement along the train consist.* Accident Analysis and Prevention, 2011. **43**(3): p. 613-620.
11. Bagheri, M., F. Saccomanno, and L. Fu, *Modeling hazardous materials risks for different train make-up*

plans. Transportation Research Part E: Logistics and Transportation Review, 2012. **48**(5): p. 907-918.
12. Rahbar, M. and M. Bagheri, *Risk Assessment Framework for the Rail Transport of Hazardous Materials:Formulation and Solution.* Transportation Research Record, 2014. **2411**(1): p. 90-95.
13. Cheng, J., M. Verma, and V. Verter, *Impact of train makeup on hazmat risk in a transport corridor.* Journal of Transportation Safety and Security, 2017. **9**(2): p. 167-194.
14. Hosseini, S.D. and M. Verma, *A Value-at-Risk (VAR) approach to routing rail hazmat shipments.* Transportation Research Part D: Transport and Environment, 2017. **54**: p. 191-211.
15. Hosseini, S.D. and M. Verma, *Conditional value-at-risk (CVaR) methodology to optimal train configuration and routing of rail hazmat shipments.* Transportation Research Part B: Methodological, 2018. **110**: p. 79-103.
16. Hosseini, S.D. and M. Verma, *Equitable routing of rail hazardous materials shipments using CVaR methodology.* Computers and Operations Research, 2021. **129**.
17. Lin, B., et al., *Integrating traffic routing optimization and train formation plan using simulated annealing algorithm.* Applied Mathematical Modelling, 2021. **93**: p. 811-830.
18. Lin, C.Y., et al., *General Model of the Effect of Hazardous Materials Car Placement in Trains and their Probability of Derailment*, in *Transportation Research Record*. 2022, SAGE Publications Ltd. p. 28-37.
19. Kang, D., et al., *Quantifying the Influence of Tank Car Position and Train Configuration on the Risk of Rail Transport of Class 3 Flammable Liquids.* Transportation Research Record, 2024.
20. Fang, K., et al., *A value-at-risk based approach to the routing problem of multi-hazmat railcars.* European Journal of Operational Research, 2025. **320**(1): p. 132-145.