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Deploying hybrid modelling to support the development of a digital twin for supply chain master planning under disruptions

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ABSTRACT

Supply chains operate in a highly disruptive environment where a SC master plan should be updated in line with disruptions to ensure that a high service level is provided to customers while total cost is minimised. There is an absence of knowledge of how a SC master plan should be updated to cope with disruptions using hybrid modelling. To fill this gap, we present a hybrid modelling framework to update a SC master plan in presence of disruptions. The proposed framework, which is a precursor to a SC digital twin, integrates simulation, machine learning, and optimisation to identify the production, storage, and distribution values that maximise SC service level while minimising total cost under disruptions. This approach proves effective in a SC disrupted by demand increase and lead time extension. Results show that employing hybrid modelling leads to a noticeable improvement in service level and total cost. The outcome of the new knowledge on using hybrid modelling for managing disruptions provides essential learning for the extension of modelling through a digital twin for SC master planning. We observe that in the presence of disruptions it is more economical to keep higher inventory at downstream SC members than the upstream SC members.

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1. Introduction

Supply chain (SC) disruptions are low-frequency-high-impact events that disrupt product, information and financial flows within a SC network (Ivanov et al. 2019). The disruptions may be caused by internal problems such as supplier failure or external events such as the Covid-19 pandemic (Badakhshan and Ball 2023). SC disruptions result in delivery delays and product shortages that propagate downstream of the SCs. This phenomenon is known as the ripple effect and adversely impacts the service level of the SCs (Dolgui and Ivanov 2021). The ripple effect occurs when a disruption is not contained in one part of a SC and spreads throughout a SC which results in a reduced service level (Dolgui, Ivanov, and Sokolov 2018). SC disruptions are becoming more prevalent. SC monitoring platform Resilinc reported that disruptions increased by 67% in 2020 compared to 2019 (Resilinc 2021). The Covid-19 pandemic was reported the most disruptive event of 2020. The demand for many products significantly increased. While the distribution lead time between SC members was extended due to delays at international borders. These led to reduced service levels (Burgos and Ivanov 2021; Ivanov and Das 2020).

Under these circumstances updating a SC master plan which contains the optimal production, storage, and distribution decisions in a SC in line with disruptions is key to minimising the impact of the disruptions on the SC service level. To identify these decisions, SC planners need to consider the complex dynamic interactions between a wide range of variables in the presence of disruptions (e.g. demand growth, lead time extension) which may result in an intractable problem (Bis-chak et al. 2014). To address this, modelling techniques that efficiently capture the complexities and dynamic behaviour of SCs need to be integrated with the modelling techniques that can identify the optimal configurations (Ivanov and Dolgui 2021; Serrano-Ruiz, Mula, and Poler 2021). Additionally, such configurations would be used for analysing real-time or near real-time data that are collected in a SC digital twin.

Simulation models have been widely applied to investigate the impact of disruptions on SC performance, owing to their capability in capturing complexities and incorporating the dynamic behaviour of SCs (e.g. Ivanov 2020; Li and Zobel 2020; Llaguno, Mula, and Campuzano-Bolarin 2022; Olivares-Aguila and ElMaraghy 2021). The main shortcoming of the simulation

models is that they compare the effects of varied decisions on SC performance under disruptions through performing what-if analysis and are not able to guide the decision makers by generating decision rules (Badakhshan et al. 2020). Machine learning can address this shortcoming as it is able to assist decision makers in identifying suitable decisions in presence of disruptions by generating decision rules (Priore et al. 2019). The application of machine learning for predicting and managing disruptions has been sparse (e.g. Brintrup et al. 2020; Zheng, Kong, and Brintrup 2023). Although, it has been widely used for demand forecasting in SCs (e.g. Guo et al. 2022; Kantasa-Ard et al. 2021; Lau, Zhang, and Xu 2018; Zhu et al. 2021). Simulation and machine learning are predictive tools, therefore they cannot identify the optimal SC master plan i.e. the optimal production, storage, and distribution decisions (Ball and Badakhshan 2021).

Optimisation models are prescriptive tools which can identify an optimal SC master plan and have been widely used in the literature (e.g. Arani and Torabi 2018; Sutthibutr and Chiadamrong 2019; Yaghin, Sarlak, and Ghareaghaji 2020). These models are not as efficient as simulation models in capturing complexities and incorporating the dynamic behaviour of SCs as considering these significantly increases their computational time. Moreover, optimisation models only identify the optimal decisions and do not generate decision rules as machine learning does to assist decision makers in the decision-making process.

By integrating simulation, optimisation, and machine learning techniques, we can reap the benefits of each technique. There is a gap in research on integrating simulation, optimisation, and machine learning for SC master planning. Moreover, there is a gap in the SC master planning literature of considering disruptions. From this perspective, this work develops a hybrid modelling framework which integrates simulation, optimisation, and machine learning for SC master planning under lead time and demand disruptions. A SC digital twin which is a replication of the physical supply chain in digital environment is an effective tool for minimising the impact of disruptions on SC performance. The reason for this is that a SC digital twin is responsive to disruptions and updates SC decisions in line with disruptions. Hybrid modelling is one of the main precursors to a SC digital twin. The hybrid modelling frameworks are needed to show the functionality of digital twins offline before their integration with real-time or near real-time data can be attempted. Leaping at live data directly without solving the underlying modelling challenges will mean that whilst real-time or near real-time modelling can be carried out, it is insufficient to address

SC master planning problem under disruptions in a reasonable time. Although, literature on digital twins for productions have highlighted the significance of hybrid modelling frameworks that incorporate simulation, optimisation, and machine learning for tackling SC master planning problem under disruptions (e.g. Dolgui, Ivanov, and Sokolov 2020; Ivanov and Dolgui 2021), no studies have demonstrated the application of such hybrid frameworks in practice. To fill this gap, this study presents a hybrid modelling framework that combines simulation, optimisation, and machine learning to address the SC master planning problem in presence of demand and lead time disruptions. The research contribution therefore is demonstrating the ability to generate optimised, explainable solutions with decision rules that account for dynamics, constraints and disruptions in both demand and lead time with a single framework.

The developed framework aims to answer three research questions: (1) What is the impact of disruptions on SC service level? (2) How can a hybrid modelling framework identify an optimal SC master plan to maximise SC service level in the presence of disruptions while minimising SC total cost? and (3) How can a hybrid modelling framework support the development of a SC digital twin? By addressing these research questions, it is possible to both understand and minimise the impact of disruptions giving the potential for identifying the optimal SC master plan in the presence of disruptions which in turn improves the service level. To answer the first question, the framework uses discrete-event simulation (DES) which is a widely used tool for examining the impact of disruptions on SC performance. To answer the second question, the framework integrates simulation, optimisation, and machine learning to update a SC master plan according to disruptions. Hybrid modelling is more efficient than individual simulation, optimisation, and machine learning for answering research question 2 as it overcomes the shortcoming of being bound by underlying methodological constraints that exist in each of these modelling approaches (Onggo et al. 2018). Simulation and machine learning cannot determine an optimal SC master plan to maximise SC service level under disruptions while minimising SC total cost because they are predictive tools not prescriptive ones. Optimisation is a prescriptive tool which can identify an optimal SC master plan to maximise SC service level under disruptions while minimising SC total cost but incorporating SC dynamics significantly increases its computational time. By integrating simulation, optimisation, and machine learning we can identify an SC master plan which minimises SC total cost and maximises SC service level under disruptions in a reasonable time.

To answer the third question, the role of the developed framework in a SC digital twin is discussed. Hybrid modelling is the backbone of a SC digital twin. The hybrid modelling frameworks are needed to demonstrate the functionality of digital twins offline before their integration with real-time or near real-time data can be attempted. Rushing into using live data without addressing the underlying modelling challenges will mean that whilst real-time or near real-time modelling can be conducted it is insufficient to address SC master planning problem under disruptions in a reasonable time.

To illustrate the effectiveness of our approach, we compare its performance against the case in which the SC master plan is not adjusted in line with disruptions. This study aims to show that hybrid modelling can support decision making better than one technique alone and therefore would result in increased performance. In turn, the proposed hybrid modelling framework may contribute to the development of a SC digital twin by incorporating real-time or near real-time data on the product and order flows.

The remainder of the paper is organised as follows: the literature review is presented in Section 2. Section 3 describes the SC master planning problem under disruptions and presents the hybrid modelling framework for addressing the problem. Section 4 discusses the impacts of three disruption scenarios on the SC service level. Section 5 shows the performance of the hybrid modelling framework in managing the disruptions. Section 6 discusses the role of the hybrid modelling in a SC digital twin. Finally, Section 7 identifies the contributions to knowledge and presents further research directions.

2. Literature review

The literature review is organised in line with four research domains that are relevant to this study. These are hybrid modelling for SC planning, SC disruption management, SC master planning and digital twins for production. For each of these reviews searches were based on Boolean combinations of keywords in specific databases and generic inclusion and exclusion criteria were applied. Throughout the Scopus data was used. For the hybrid modelling review, the Web of Science and IEEE Xplore databases were also employed. The inclusion criteria were manufacturing supply chains, empirical studies (either real case study or using synthetic datasets) and planning applications. The exclusion criteria were theoretical studies, studies without application, those not primarily focused on planning, absence of data sourcing and lack of actionable decisions. The papers were drawn exclusively from the keyword search and snowballing was not used.

2.1. Hybrid modelling for SC planning

Hybrid modelling refers to a modelling approach which consists of more than one modelling technique. The use of hybrid modelling for addressing SC planning problems has gained popularity among both researchers and practitioners (Mustafee et al. 2017). The reason for this is that the hybrid modelling approach overcomes the shortcoming of being bound by underlying methodological constraints that exist in a single modelling approach (Onggo et al. 2018). Of particular interest in this study is the integration of simulation, optimisation, and machine learning techniques for SC planning and the gaps in these techniques to address SC planning problems. Therefore, we review previous studies which have integrated these techniques to address SC planning problems. The search was used keywords 'simulation', 'optimisation', 'machine learning', and 'supply chain'. The identified papers were then reviewed and those in which there was a clear data exchange between the modelling techniques were selected. Table 1 presents a summary of the literature on hybrid modelling for SC planning.

The first group of papers integrated simulation and optimisation to address SC planning problems. These papers use simulation for considering SC uncertainties and optimisation for determining optimal SC decisions. For instance, Clavijo-Buritica, Triana-Sanchez, and Escobar (2022) and Akhtari and Sowlati (2020) integrated a discrete-event simulation (DES) model and a mixed-integer programming (MIP) model to address a SC network design problem. The DES model investigated the impact of disruptions on SC performance and the MIP model identified the optimal production, storage and distribution values. Safaei et al. (2010) and Bilgen and Çelebi (2013) paired a DES model which was responsible for handling uncertainties such as machine breakdowns, queuing, and transportation delays and a MIP model which determined the optimal decisions to address a production-distribution planning problem. The main shortcoming of these papers is that they do not provide any insight into the process of identifying the optimal SC decisions. To overcome this shortcoming, clear-box algorithms which can provide insight into decision-making process by generating decision rules are needed.

The second group of studies integrated simulation and machine learning to address SC planning problems. These studies use simulation data for training machine learning algorithms. Jackson and Velazquez-Martinez (2021) employed a DES model to generate data for a multilayer perceptron model which classified inventory policies as profitable or non-profitable in a food SC. Morin et al. (2020) used the generated data by sawing

Table 1. Literature on hybrid modelling for SC planning.

Study	Hybrid modelling approach	Simulation role	Optimisation role	Machine learning role
Clavijo-Buritica, Triana-Sanchez, and Escobar (2022), Akhtari and Sowlati (2020)	Simulation-optimisation	Predict the impact of disruptions on SC performance	Optimise SC network design	-
Safaei et al. (2010) and Bilgen and Çelebi (2013)	Simulation-optimisation	Handle SC uncertainties	Optimise production and distribution decisions	-
Jackson and Velazquez-Martinez (2021), Morin et al. (2020), Cavalcante et al. (2019), Badakhshan and Ball (2023) and Priore et al. (2019)	Simulation-machine learning	Generate data	-	Predict SC performance
Islam, Amin, and Wardley (2021)	Optimisation-machine learning	-	Optimise supplier and order allocation	Predict uncertain parameters in optimisation model
Gumte et al. (2021)	Optimisation-machine learning	-	optimise SC network design	Predict uncertain parameters in optimisation model
Bhosekar and Ierapetritou (2021), Goettsch, Castillo-Villar, and Aranguren (2020)	Optimisation-machine learning	-	Optimise SC network design	Shrink the decision space
Onggo et al. (2018) and Onggo (2019), Pereira and Frazzon (2021), Raghuram et al. (2022), Gonzalez, Jalali, and Van Nieuwenhuysse (2020)	SBO-machine learning	Estimate optimisation objective	Optimise simulation parameters	Predict uncertain parameters in simulation model

simulation to train machine learning models to predict the baskets of products that could be produced from a log. Cavalcante et al. (2019) paired simulation and machine learning to address a supplier selection problem. Badakhshan, Ball, and Badakhshan (2022) and Priore et al. (2019) trained a decision tree algorithm using simulation data to reduce the bullwhip effect and cash flow bullwhip in SCs, respectively. The main limitation of these papers is that they cannot identify the optimal SC decisions. In other words, they are only predictive and not prescriptive. To address this limitation, optimisation models are needed to determine the optimal SC decisions.

The third group contains papers that integrated optimisation and machine learning. Some of these papers employ machine learning for predicting uncertain parameters in optimisation models. For instance, Islam, Amin, and Wardley (2021) paired a MIP model and the relational regression chain method to address a supplier selection and order allocation problem. Gumte et al. (2021) employed the Neuro-Fuzzy C-means clustering algorithm to handle uncertainty in a robust optimisation model which was developed for a biomass SC network design. Some papers used machine learning to shrink the decision space of an optimisation model and therefore reduce the computation time. Bhosekar and Ierapetritou (2021) employed the support vector machine method to approximate feasible production

regions in a MIP model which aimed to optimise a modular manufacturing SC. Goettsch, Castillo-Villar, and Aranguren (2020) employed a multilayer perceptron model to select potential depots in a MIP model which aimed to optimise a biomass SC. The main limitation of these papers is that they mostly used black-box machine learning algorithms which are unable to generate decision rules for the decision makers. To address this limitation, again clear-box machine learning algorithms are needed to generate decision rules for the decision makers.

The fourth group contains studies that integrated simulation-based optimisation (SBO) and machine learning. SBO is a modelling framework which incorporates an optimisation algorithm into a simulation model to determine the optimal simulation parameters configuration (Kück et al. 2016). In SBO, the optimisation objective function is estimated using a simulation model (Aslam and Ng 2015). These studies used machine learning to predict uncertain parameters in simulation models. Onggo et al. (2018) and Onggo (2019) developed conceptual frameworks for integrating machine learning and SBO. Pereira and Frazzon (2021) and Raghuram et al. (2022) presented a two-step approach for synchronising demand and supply in SCs. In the first step, demand was forecasted using an artificial neural network. In the second step, the forecasted demand was inputted into an SBO model where optimal distribution

and inventory parameters were identified using an optimisation algorithm. Gonzalez, Jalali, and Van Nieuwenhuyse (2020) used a gaussian process regression model to improve search efficiency in an SBO model. These studies use SBO to determine the optimal values of the decision parameters in SCs. The limitation of the SBO is that it cannot include constraints on decision variables such as the flow of products in a SC and therefore it cannot identify the optimal values for the decision variables. This is because decision variables are endogenous to simulation. To determine the optimal values for the decision variables, there needs to be an independent optimisation model which contains constraints on the decision variables. To this end, an independent optimisation model, e.g. MIP, is needed to determine the optimal decisions in a SC. Moreover, these studies used machine learning only for predicting uncertain parameters in a simulation model. Machine learning could also be used for defining constraints on the decision variables in an optimisation model.

Much of the literature on hybrid modelling for SC planning do not consider disruptions. Moreover, there is a scarcity of studies that show the application of a simulation-optimisation-machine learning framework to address SC planning problems. Although the applications of such frameworks in other domains have been presented (e.g. Dong et al. 2022; Harper and Mustafee 2019; Hou et al. 2022; Mohammadi, Safari, and Vazifekhhah 2022). Therefore, there is a gap in the literature on the application of a simulation-optimisation-machine learning framework to address SC planning problems under disruptions. This confirms research question 2: How can a hybrid modelling framework identify an optimal SC master plan to maximise SC service level in the presence of disruptions while minimising SC total cost? To address these gaps, a combination of simulation, optimisation, and machine learning offers an opportunity to address a SC master planning problem in the presence of demand and lead time disruptions. There is the potential for strengths in each technique to overcome the weaknesses in other techniques.

2.2. SC disruption management

The existing body of literature on SC disruption management has employed various modelling approaches to develop strategies aimed at reducing the adverse effects of disruptions on SC performance. Simulation is widely used to investigate the impact of disruptions on SC performance, owing to its capability in capturing complexities and incorporating the dynamic behaviour of SCs (Ivanov and Dolgui 2021). The first category shown in Table 2 corresponds to studies which applied simulation

for modelling SC disruptions. Three main simulation methods, namely discrete-event simulation (DES), system dynamics (SD), and agent-based simulation (ABS) have been utilised to model SC disruptions.

For instance, Carvalho et al. (2012) investigated the impact of transportation disruption on SC total cost. They suggested holding redundant inventory and having back-up transport could serve as effective strategies to mitigate the impact of transportation disruption. Ivanov (2020) considered supply, transportation, and demand disruptions to study the impact of COVID-19 on global supply chains. Olivares-Aguila and ElMaraghy (2021) and Llaguno, Mula, and Campuzano-Bolarin (2022) examined how supply and production capacity disruptions affect the profitability and service level of SCs. Bueno-Solano and Cedillo-Campos (2014) explored the effects of border disruptions on inventory levels and total costs within a global automotive supply chain. Chauhan, Perera, and Brintrup (2021) created a model for the propagation of failures to examine how a nested pattern topology affects the resilience of SCs in the face of supply disruptions. Li and Zobel (2020) introduced a framework for assessing the resilience of a supply chain when confronted with the ripple effect which refers to the disruption propagation from the initial disruption point throughout the SC (Ivanov et al. 2019). The main limitation of these studies is that they cannot optimise SC performance. To address this, they need to be integrated with an optimisation technique.

The second category of papers used machine learning to predict disruptions and mitigate the negative impact of disruptions on SC performance. For instance, Brintrup et al. (2020) employed a random forest algorithm to predict SC disruptions using historical data available to an Original Equipment Manufacturer (OEM). Xu, Mak, and Brintrup (2021) proposed the use of bots to reconfigure SCs in the face of disruptions. Hosseini and Ivanov (2022) developed a multilayer Bayesian network (BN) model capable of detecting triggers that caused disruptions in SCs during the COVID-19 pandemic. Zheng, Kong, and Brintrup (2023) used a federated learning approach to predict order delays in SCs. Machine learning models cannot optimise SC performance in presence of disruptions unless they are coupled with optimisation.

The third category consists of studies that applied optimisation to minimise the impact of disruptions on SC performance. Sawik (2023) presented a stochastic mixed integer programming model to address a SC reshoring problem in the presence of manufacturing, transportation, and demand disruptions. Pathy and Rahimian (2023) used optimisation to identify the optimal procurement and inventory decisions for a pharmaceutical SC under demand disruptions. Babaei, Khedmati,

Table 2. Literature on SC disruption management.

Study	Modelling approach	Disruption type	Limitation by category
Carvalho et al. (2012)	DES	Transportation	Incapable of optimising SC performance in the presence of disruptions
Ivanov (2020)	DES	Supply Transportation Demand Supply	
Olivares-Aguila and ElMaraghy (2021); Llaguno, Mula, and Campuzano-Bolarin (2022)	SD	Capacity Supply Border Supply Node Environmental Supply	
Bueno-Solano and Cedillo-Campos (2014)	SD		
Chauhan, Perera, and Brintrup (2021)	ABS		
Li and Zobel (2020)	ABS		
Brintrup et al. (2020); Xu, Mak, and Brintrup (2021); Hosseini and Ivanov (2022); Zheng, Kong, and Brintrup (2023)	Machine learning		Incapable of optimising SC performance in the presence of disruptions
Sawik (2023)	Optimisation	Manufacturing	Computationally inefficient in case of considering SC dynamics
Pathy and Rahimian (2023)	Optimisation	Transportation Demand Demand Supply	
Babaei, Khedmati, and Akbari Jokar (2023); Mohammed et al. (2023)	Optimisation	Transportation Capacity Capacity	
Wang and Yao (2023)	Optimisation		
Ivanov (2019)	DES		Not considering both demand and lead time disruptions
Ivanov and Rozhkov (2020)	Linear programming DES ABS Parametrical optimisation	Capacity	
Jaenichen et al. (2022)	Simulation Machine learning	Demand	
Sindhwani, Jayaram, and Saddikuti (2023)	Bayesian network DES Optimisation	Supply	
Saputro, Figueira, and Almada-Lobo (2021)	DES Optimisation	Supply	

and Akbari Jokar (2023) and Mohammed et al. (2023) employed optimisation to address the SC network design problem in the presence of supply disruptions. Wang and Yao (2023) optimised a SC network structure under capacity and transportation disruptions. The primary constraint of optimisation models is that they will become computationally inefficient if they consider SC dynamics as simulation and machine learning models do. To address this, optimisation models should be integrated with simulation and machine learning.

Category four includes studies that used hybrid modelling for SC disruption management. Ivanov (2019) combined DES and linear programming to address a network design and production-ordering management problem in a beverage SC in the presence of capacity disruption. Ivanov and Rozhkov (2020) integrated DES, ABS, and parametrical optimisation to address an inventory and production planning problem under capacity disruption. Jaenichen et al. (2022) investigated the

consequences of demand disruption in semiconductor SCs by combining simulation and tree-based supervised machine learning. Sindhwani, Jayaram, and Saddikuti (2023) integrated Bayesian network modelling, DES, and optimisation to mitigate the ripple effect in a pharmaceutical SC. Saputro, Figueira, and Almada-Lobo (2021) used simulation-optimisation to address an integrated supplier selection and inventory management problem in the face of supply disruptions. The main limitation of these studies is that they either consider supply or demand disruptions. There is no study which considers both demand and supply disruptions.

As per the hybrid modelling review, this SC disruption review revealed there is no study which presented a hybrid framework including simulation, optimisation, and machine learning to address a SC master planning problem in the presence of demand and lead time disruptions. This confirms research question 2: How can a hybrid modelling framework identify an optimal SC

master plan to maximise SC service level in the presence of disruptions while minimising SC total cost? To fill this gap in the SC disruption management literature, we integrate simulation, optimisation, and machine learning to address a SC master planning problem in a two-echelon SC under demand and lead time disruptions.

2.3. SC master planning

SC master planning aims to coordinate production, storage, and distribution in a SC to meet customer demand at the minimum cost. To this end, it integrates planning of different functional areas to identify the optimal

Table 3. Literature on SC master planning.

Study	Modelling approach	Model objectives	Uncertain parameters	Uncertainty handling method
Arani and Torabi (2018)	Mixed integer linear programming (MILP)	Max net present value (NPV)	Costs	Fuzzy programming
Fallah, Eskandari, and Pishvaei (2018)	MILP	Min total cost	Price Production capacity Maximum allowed debt Costs	Robust optimisation
Yaghin, Sarlak, and Ghareaghaji (2020)	Mixed integer non-linear programming (MINLP)	Max total profit	Demand Production capacity Costs	Fuzzy programming
Martín, Díaz-Madroño, and Mula (2020)	MILP	Max total cost	Price Production capacity Safety stocks Process times	Robust optimisation
Peidro et al. (2012)	LP	Max total gross margin Min idle time Min backorder	Gross margin Idle time backorder	Fuzzy programming
Sutthibutr and Chiadamrong (2019)	LP	Min total cost	Costs	Fuzzy programming
Chern, Lei, and Huang (2014)	MILP	Maximise total value of purchasing	Demand	
Gallego-García, Gallego-García, and García-García (2021)	Simulation	Min costs, Min substitution priority Max service level	Production capacity Recycling time Supply shortage	Stochastic programming Scenario analysis
Ewen et al. (2017)	Simulation	Min total cost Max production capacity	Demand	Scenario analysis
Orcun and Uzsoy (2011)	Simulation	Min Bullwhip effect	Production capacity	Scenario analysis
Powell Robinson Jr, Sahin, and Gao (2008)	Simulation	Min cost	Master plan design factors	Scenario analysis
Alves and Mateus (2020)	Machine learning	Min instability	Environmental factors	
Kegenbekov and Jackson (2021)	Machine learning	Min total cost	Demand	Markov decision process
Lauer, Legner, and Henke (2019)	Machine learning	Min bullwhip effect	Demand	Markov decision process
Afridi et al. (2020)	Machine learning	Min instability	Demand	-
Vieira et al. (2022)	Simulation-optimisation	Max service level	Demand	Markov decision process
Chern, Chen, and Huang (2014)	Simulation-optimisation	Min inventory cost Min total cost	Processing and setup times Robot travelling velocity Recycling time Processing and setup times	Simulation
Li et al. (2016)	Simulation-optimisation	Max total profit Max fill rate		Simulation
Nedaei and Mahlooji (2014)	Simulation-optimisation	Min cost	Demand Master plan design factors	Simulation
		Min instability	Environmental factors	

production, storage and distribution values in a SC (Pibernik and Sucky 2007). Previous studies have mostly employed one modelling technique to address the SC master planning (SCMP) problem. Table 3 presents a summary of the literature on SCMP.

The first cluster of papers developed optimisation models to address the SCMP problem. For instance, Arani and Torabi (2018) presented a bi-objective mixed possibilistic-stochastic model to address a SCMP problem that integrated physical and financial flows. Sutthibutr and Chiadamrong (2019) presented a multi-objective linear fuzzy model to identify an optimal SC master plan in an uncertain environment. Yaghin, Sarlak, and Ghareaghaji (2020) proposed a mixed-integer non-linear programming model to deal with the master planning of a socially sustainable SC under fuzzy-stochastic uncertainty. Social sustainability was investigated through the lens of workers' working conditions and social investment. Martín, Díaz-Madroñero, and Mula (2020) addressed a SCMP problem for a second-tier automobile supplier using robust optimisation.

The second cluster contains studies that employed simulation to study a SCMP problem. Gallego-García, Gallego-García, and García-García (2021) presented a simulation model to identify the best-fit procurement order quantities for a manufacturer that faced supply shortages from his supplier. Ewen et al. (2017) proposed a simulation model to determine strategies for improving manufacturing capacity in semiconductor SCs. Orcun and Uzsoy (2011) used system dynamics simulation to study the effects of SC master planning on the dynamic behaviour of the SCs. Powell Robinson Jr, Sahin, and Gao (2008) applied simulation to evaluate the impact of four SC master plan design factors including non-frozen interval policy, planning horizon length, frozen interval length and re-planning frequency and four environmental factors including natural order cycle length, vendor flexibility, demand range and demand lumpiness on cost and instability of the SC master plan.

The third cluster includes studies that employed machine learning techniques to address a SC master planning problem. For instance, Alves and Mateus (2020) and Kegenbekov and Jackson (2021) applied the proximal policy optimisation algorithm which is a deep reinforcement learning algorithm to deal with the SC master planning problem under demand uncertainty. Lauer, Legner, and Henke (2019) employed the random forest algorithm to predict the instability of a master plan in a semiconductor SC. Afridi et al. (2020) used the Q-learning algorithm to find the optimal replenishment policy under a vendor-managed inventory setting in a semiconductor SC.

Finally, cluster four contains studies that used simulation-optimisation to address a SCMP problem. Ponsignon and Mönch (2014) presented a simulation-optimisation model that integrated discrete-event simulation and genetic algorithms to determine the optimal master plan in a semiconductor SC. Chern, Chen, and Huang (2014) coupled a heuristic algorithm called stochastic recycling process planning algorithm (SRPPA) with simulation to address a SCMP problem in a recycling supply chain. Li et al. (2016) integrated a metamodel-based Monte Carlo simulation with multi-objective optimisation to address a SC master planning problem. Vieira et al. (2022) proposed a simulation-optimisation approach that integrated a two-level mixed integer linear programming model and a discrete-event simulation model to determine the optimal master plans in a SC.

There is no study on addressing the SCMP problem in the presence of demand and lead time disruptions. This confirms research question 1: What is the impact of disruptions on SC service level? Moreover, Serrano-Ruiz, Mula, and Poler (2021) presented a conceptual framework in which they highlighted the need for an integrated simulation-optimisation-machine learning framework to address a SC master planning problem in the face of disruptions. Although, there is no study which showed the application of such an integrated framework for addressing a SCMP problem in practice. This confirms research question 2: How can a hybrid modelling framework identify an optimal SC master plan to maximise SC service level in the presence of disruptions while minimising SC total cost? To fill these gaps in the literature, we integrate simulation, optimisation, and machine learning to address a SCMP problem in a two-echelon SC under demand and lead time disruptions.

2.4. Digital twins for production

A digital twin is a virtual representation of a physical product or system that mirrors its physical counterpart. To achieve this, the digital twin should have real-time or near real-time communication with its physical twin throughout its lifecycle (Grieves and Vickers 2017). A digital twin evaluates the performance of its physical counterpart and generates valuable insights to improve its performance. Digital twin development provides cost saving opportunities such as reducing defects and improving production efficiency (Badakhshan and Ball 2021). The seven major elements of a digital twin in SC and operations management are defined as technology, people, management, organisation, scope, task, and modelling (Ivanov 2023a). Researchers have developed digital twins of products and systems throughout

four phases of their lifecycle including design, manufacturing, service, and retirement. The design phase refers to the design of products and manufacturing processes and systems. The manufacturing phase includes the production and internal plant logistics. The service phase contains distribution, use, and repair. The retirement phase comprises operations such as disassembling, remanufacturing, reusing, and disposal. Much of the literature on digital twins for production employed simulation and optimisation modelling. Table 4 presents a summary of the literature on the application of digital twins in production systems.

The first set of papers developed digital twins in the design phase of the physical twin's lifecycle. For instance, Huang, Wang, and Yan (2022) developed a digital twin of reconfigurable machine tools to reduce manufacturing cost. Sharma (2023) used a digital twin of a Cobotic inspection work cell to reduce inspection time and error in electric vehicle battery assembly process. Tao et al. (2019) presented a digital twin-driven framework for product design to reduce the design cost and design cycle for a bicycle manufacturer. Liu et al. (2019) developed a digital twin of a shop floor manufacturing system to examine the performance of the system before production. Aderiani et al. (2019) used a digital twin to find the optimal combinations of individual parts in the design process of sheet metal assemblies. These studies concentrate on minimising design cost of manufacturing products and processes and do not consider SC disruptions.

The second set of studies focused on the manufacturing phase of the physical twin's lifecycle. Ding et al. (2019) proposed a digital twin cyber-physical production framework for production planning and control. Zhang et al. (2022) presented an improved multi-fidelity simulation-optimisation to reduce the computational time of large-scale discrete optimisation problems that are developed for production planning and control in a digital twin shop floor. Ait-Alla et al. (2021) employed simulation-optimisation approach to optimise the interconnection between a production system and its digital twin. Leiden, Herrmann, and Thiede (2020) developed a digital twin to increase the efficiency of energy and resource planning in the Zinc nickel electroplating process chain. Sharma and Kumar Tiwari (2022) presented digital twins of robotic work cells to scale up cost-effective assembly of electric vehicle battery. Wang, Lee, and Angelica (2021) developed a digital twin of a die-cutting machine to monitor machine conditions in real-time. These studies focus on minimising the impact of production disruptions at manufacturer and do not study the impact of disruptions at SC level.

The third set of papers studied the service phase of the physical twin's lifecycle. These studies investigated the role of SC digital twins in managing disruptions. SC Digital twins can simulate different scenarios to evaluate the impact of disruptions such as supplier delays, transportation disruptions, or changes in customer demand on SC performance. By modelling these disruptions, companies can assess the potential consequences and explore alternative courses of action. This helps in developing contingency plans and making proactive decisions to mitigate the impact of disruptions. Burgos and Ivanov (2021) used a SC digital twin to assess the impact of COVID-19 on food retail SCs. Park, Son, and Noh (2021) presented a digital twin-based SC control framework to minimise bullwhip effect and ripple effect in an automobile parts SC. Badakhshan and Ball (2023) presented a SC digital twin framework for inventory and cash management under physical and financial disruptions. Zdolsek Drakslar, Cimperman, and Obrecht (2023) developed a SC digital twin to tackle a last mile delivery problem in the presence of transportation disruptions. The main shortcoming of these studies is that they used either simulation or coupled simulation with machine learning to manage disruptions. These studies cannot optimise SC performance in the presence of disruptions due to the nature of simulation and machine learning, which are primarily predictive rather than prescriptive.

SC digital twins can incorporate risk assessment models to identify potential vulnerabilities in the SC. By analysing historical data, market trends, and external factors, SC digital twins can assess the probability and impact of disruptions. This information allows companies to prioritise risk mitigation efforts and allocate resources effectively. Ivanov and Dolgui (2021) explored the conditions surrounding the design and implementation of the digital twins for managing disruption risks and improving resilience in SCs. Dolgui, Ivanov, and Sokolov (2020) introduced the concept of reconfigurable SCs or the X-network to integrate digitalisation, resilience, sustainability, and leagility (Dolgui, Ivanov, and Sokolov 2018) in SCs. Ivanov (2023b) proposed a human-AI system called intelligent digital twin for SC stress-testing and resilience. Ivanov and Dolgui (2022) conceptualised the application of SC digital twins for preventing the ripple effect in SCs. Serrano-Ruiz, Mula, and Poler (2021) presented a conceptual framework in which they discussed the role of SC digital twins in addressing master production scheduling problem in the presence of disruptions. These studies presented conceptual frameworks but did not show the application of SC digital twins in practice.

In the absence of hybrid models that integrate simulation, optimisation, and machine learning, a SC digital twin is limited by the inherent methodological

Table 4. Review of digital twins in production.

Study	Lifecycle phase	Research scope	Modelling approach	Business outcome	Case study
Sharma (2023)	Design	Process design	Simulation	Reducing inspection time and error	Electric vehicle battery assembly
Huang, Wang, and Yan (2022)	Design	Product and process design	Machine Learning Simulation	Reducing manufacturing cost	Reconfigurable machine tools
Tao et al. (2019)	Design	Product design	Simulation	Design cost and design cycle reduction	Bicycle design
Liu et al. (2019)	Design	Product and process design	Data mining Simulation	Design cost reduction	Sheet metal assembly
Aderiani et al. (2019)	Design	Product design	Optimisation Simulation	Increasing the geometrical quality of final product	Sheet metal assembly
Zhang et al. (2022)	Manufacturing	Production planning and control	Optimisation Simulation	Reducing the computational time	Aircraft parts
Ding et al. (2019)	Manufacturing	Production planning and control	Optimisation Simulation	Production efficiency enhancement	General shop floor manufacturing
Ait-Alla et al. (2021)	Manufacturing	Process planning and control	Optimisation Simulation	Mean throughput time	Light
Sharma and Kumar Tiwari (2022)	Manufacturing	Process planning and control	Simulation	Resource utilisation Increasing throughput	Electric vehicle battery assembly
Leiden, Herrmann, and Thiede (2020)	Manufacturing	Energy and resource planning	Simulation	Reduce production cost Increasing resource and energy efficiency	Zinc nickel electroplating process chain
Wang, Lee, and Angelica (2021)	Manufacturing	Maintenance	Simulation	Reducing maintenance cost	Die cutting machine
Park, Son, and Noh (2021)	Service	SC planning	Simulation	Reducing bullwhip effect and ripple effect	Automobile parts SC
Ivanov and Dolgui (2021)	Service	SC planning	Simulation Optimisation Data analytics	Enhancing SC resilience	General
Serrano-Ruiz, Mula, and Poler (2021)	Service	SC planning	Simulation	Enhancing SC resilience	General
Dolgui, Ivanov, and Sokolov (2020)	Service	SC planning	Optimisation Machine learning Simulation	Enhancing SC resilience	General
Ivanov (2023b)	Service	SC planning	Optimisation Data analytics Simulation Optimisation Data analytics	SC stress-testing Enhancing SC resilience	General
Badakhshan and Ball (2023)	Service	SC planning	Simulation	Minimising cash conversion cycle	FMCG
Zdolsek Draksler, Cimperman, and Obrecht (2023)	Service	SC planning	Machine learning Simulation	Reducing SC cost	Last mile delivery
Wang and Wang (2019)	Retirement	Recovery and remanufacturing	Machine learning Simulation	Reducing electrical and electronics equipment waste	Electrical and electronic equipment
Wang et al. (2020)	Retirement	Recovery and remanufacturing	Simulation Optimisation Data analytics	Reducing the uncertainty in remanufacturing process	Automatic guided vehicle remanufacturing

constraints associated with each of these modelling approaches. Consequently, it is unable to effectively optimise SC performance in the face of disruptions.

Although, various studies presented conceptual frameworks to underline the importance of such hybrid frameworks (e.g. Dolgui, Ivanov, and Sokolov 2020; Ivanov

2023; Ivanov et al. 2019; Ivanov and Dolgui 2022; Serrano-Ruiz, Mula, and Poler 2021). There is no study that shows the practical implementation of a SC digital twin framework incorporating simulation, optimisation, and machine learning to minimise the impact of lead time and demand disruptions on SC performance. To fill this gap, we develop a SC digital twin which incorporates simulation, optimisation, and machine learning to minimise the impact of lead time and demand disruptions on SC performance.

The fourth set of studies examined the role of a digital twin in the retirement phase of a physical twin lifecycle. Wang and Wang (2019) developed a digital twin framework for the recovery and remanufacturing of retired electrical and electronic equipment. Wang et al. (2020) proposed Big Data-driven Hierarchical Digital Twin Predictive Remanufacturing paradigm to reduce uncertainty in the remanufacturing process of retired products.

The gaps in digital twins for production literature are as follows. Firstly, Literature on digital twins in production is still in its infancy and more research on the application of digital twins in practice is required (Badakhshan and Ball 2021). Secondly, much of the literature either use simulation or integrate simulation and machine learning or integrate simulation and optimisation. There is limited research on the application of hybrid modelling frameworks which integrate simulation, optimisation, and machine learning. Although the importance of such frameworks in developing SC digital twins has been highlighted in the literature (e.g. Dolgui, Ivanov, and Sokolov 2020; Ivanov 2023; Ivanov and Dolgui 2021). This confirms research question 3: How can a hybrid modelling framework support the development of a SC digital twin? Thirdly, the hybrid modelling frameworks are needed to show the functionality of digital twins offline before their integration with real-time or near real-time data can be attempted. Leaping at live data directly without solving the underlying modelling challenges will mean that whilst real-time or near real-time modelling can be

carried out it is insufficient to address SC master planning problem under disruptions in a reasonable time. Fourthly, there is no study that showed the application of digital twins to address SC master planning problem under demand and lead time disruptions in practice.

To fill these gaps, in this study, a hybrid model which integrates a simulation model, DES, an optimisation model, MIP, and a machine learning algorithm, the decision tree, is developed to minimise the impact of demand and lead time disruptions on SC service level.

2.5. Summary of literature review

There are four features that are collectively absent from the four strands of literature discussed in Sections 2.1–2.4: (a) optimisation, (b) explainable solutions with decision rules, (c) the presence of SC dynamics, and (d) demand and lead time disruptions. These four features independently exist in published works but not combined. To consider these four features simultaneously, this study presents a hybrid modelling framework which integrates simulation, optimisation, and machine learning. This hybrid framework is used to address a SC master planning problem in the presence of demand and lead time disruptions. The hybrid modelling framework uses simulation to incorporate the dynamic behaviour of SCs (feature c) under demand and lead time disruptions (feature d). It uses machine learning to provide explainable solutions (feature b) on the minimum inventory values that ensure a service level above 98% for all products. It uses optimisation (feature a) to identify the optimal production, storage, and distribution values that minimise the SC total cost.

3. Problem description and modelling approach

Following on from the literature review outcome, the problem considered here is the SC master planning. The general structure of the studied SC is depicted in Figure 1. The SC includes two echelons: (1) manufacturers, and (2)

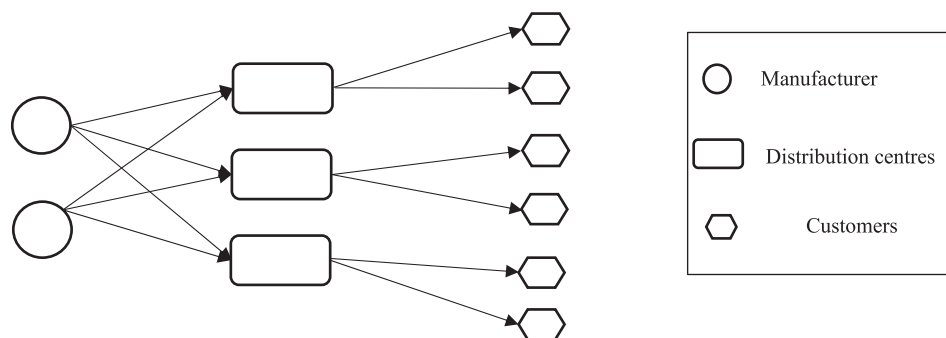


Figure 1. The general structure of the SC.

distribution centres (DCs). Manufacturers send products to DCs which are responsible for meeting the uncertain demands of end customers. In this study multiple products and periods are considered. Production capacities at manufacturers and storage capacities at distribution centres are restricted to reflect practice. This is typical of the configurations considered in the literature (e.g. Fallah, Eskandari, and Pishvae 2018; Yaghin, Sarlak, and Ghareaghaji 2020). The decisions to be addressed are: (1) The production rates at manufacturers (2) The flow of products in the network, (3) The inventory levels at SC members, (4) The number of products which have not been delivered in time to the customers, i.e. backlog, and (4) The number of the required workforce at manufacturers. We aim to minimise SC total cost by identifying the optimal values for decisions 1–4. In the presence of SC disruptions, the optimal values of decisions 1–4 need to be updated in line with the disruptions to minimise the impact of the disruptions on the SC service level. Integrating simulation, optimisation and machine learning has the potential to provide an effective way of decision making in the presence of disruptions. Therefore, in this study, we develop a hybrid modelling framework that integrates simulation, optimisation and machine learning to update the optimal values of the decision 1–4 in line with disruptions.

3.1. Hybrid modelling framework

The literature reviews earlier brought out the gaps in current disruption modelling work. This work sought to

develop and deploy a framework that could be configured to provide four simultaneous features of (a) generate explainable solutions with decision rules, (b) optimal solutions, (c) that account for system dynamics and constraints and (d) disruptions (in both demand and lead time). These four features independently exist in published works but not combined. This novelty has therefore potential to generate better, explainable, practical solutions to SCs under disruptions.

Figure 2 shows the developed hybrid modelling framework. The simulation model represents the physical SC by considering the dynamics (feature (c)) in the product and order flows under constraints and generates the inventory data to be inputted into the machine learning model. The machine learning model then generates decision rules (feature (a)) for setting the minimum inventory levels of products at SC members. The decision maker defines the minimum inventory levels of products at SC members into an optimisation model where the SC master plan is determined (feature (b)). In the presence of disruptions (feature (d)) the framework triggers the re-running of the simulation and machine learning to develop new rules for new explainable solutions.

When disruptions in product flow happen the simulation model is updated, and a new set of data is fed into the machine learning model to give new decision rules for setting the minimum inventory levels of products at SC members in optimisation model. In turn, the SC master plan which consists of the optimal production, storage and distribution decisions is outputted to the physical SC for execution. Figure 2 captures the essence

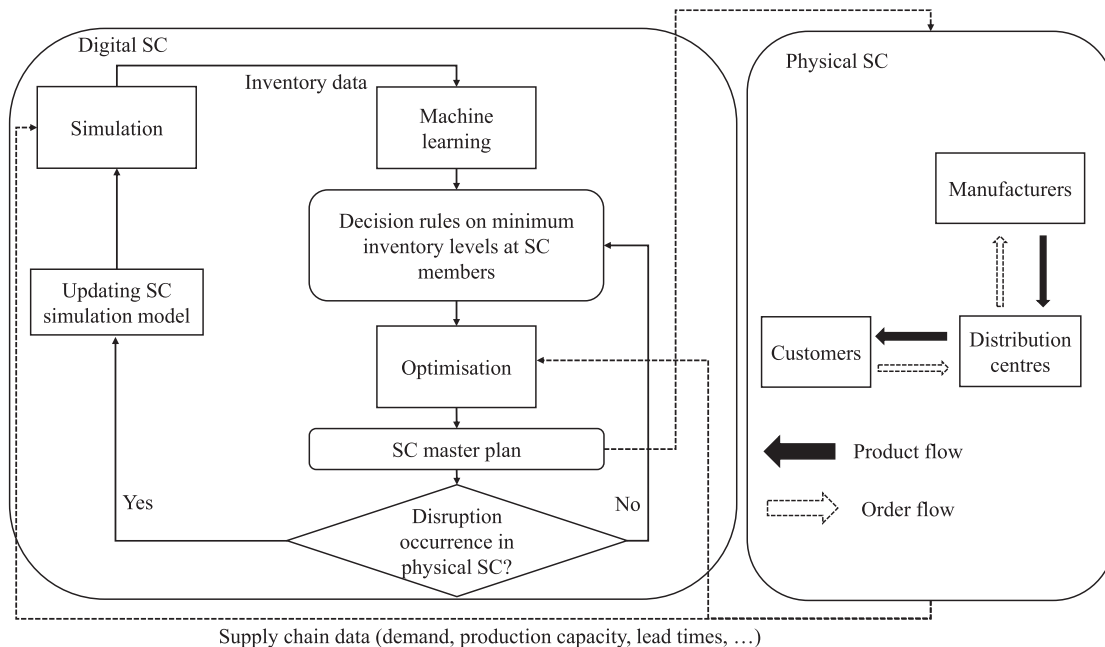


Figure 2. Hybrid modelling framework.

of digital twins with the flow of data between the physical supply chain and the digital model equivalent and back. Whilst the set up could have been for real-time continuous updates, the set up was periodic updates with specific updates when disruptions are detected. This allowed the research to incorporate the properties of digital twins with lower frequency updates but still useful for decision making.

One challenge in implementing such hybrid frameworks is interfacing simulation, optimisation, and machine learning models as these models are mostly developed using different system architectures and software. To overcome this challenge, we use Python language to develop simulation, optimisation, and machine learning models. This removed the software barrier to integration and so the focus could be on integrating the modelling conceptually.

3.1.1. Decision tree algorithms

The Decision tree is a supervised machine learning technique that discovers decision rules in the form of if-then-else statements from data. This simplifies the decision-making process for the users. The decision tree technique extracts the decision rules by inspecting a training dataset with m examples that are represented as a features-value table. The features refer to the inputs of the problem and the value refers to the output of the problem that is going to be predicted. The decision tree technique follows three steps to extract the decision rules: (1) Splitting the training dataset into n sub-tables. One table for each possible output value, (2) Dividing combinations of the features and counting the number of occurrences for each combination in the rows of the sub-tables, (3) Sorting the combinations of the features based on the number of occurrences in descending order and extracting the decision rules accordingly.

This research seeks to provide guidelines to assist decision makers in setting out minimum inventory levels of products at SC members by generating decision rules. This helps the decision makers in comprehending the decision-making process. The decision tree technique can provide decision rules, unlike most machine learning techniques which are generally considered black-box systems (Priore et al. 2019). Therefore, we employ the decision tree technique. There is a wide range of decision tree algorithms such as CART (Breiman et al. 1984), MARS (Friedman 1991), ID3 (Quinlan 1979), C4.5 (Salzberg 1994), and CHAID (Kass 1975). Among the decision tree algorithms, C4.5 and CART are the most employed owing to their capability in making a good trade-off between learning speed and error rate (AlMana and Aksoy 2014; Wu et al. 2008). Therefore, in this study, we use the CART algorithm.

The CART algorithm uses the concept of Gini impurity to sequentially select the nodes of the decision. The Gini impurity indicates the likelihood of incorrect classification of new, random data if it were given a random class label according to the class distribution in the dataset. Equation (1) defines the Gini impurity for a dataset that contains D rows and n classes.

$$Gini(D) = \sum_{i=1}^n p_i(1 - p_i) = 1 - \sum_{i=1}^n p_i^2 \quad (1)$$

where p_i represents the probability of samples belonging to class i at a given node. In the case of all records belonging to the same class, the Gini impurity would be zero. The best feature for the first split of the decision tree is determined by calculating the Gini impurity for all features and selecting the feature with the lowest Gini impurity. This process continues for each subsequent split until the maximum depth of the decision tree is reached. The maximum depth of a decision tree is a hyperparameter that could be set by the user. If the user does not specify the maximum depth of a decision, the nodes will be expanded until all leaf nodes contain only one class. More detail on the CART algorithm can be found in (AlMana and Aksoy 2014; Breiman et al. 1984; Wu et al. 2008).

3.1.2. Simulation model

As it was shown in Figure 1, in this study, a two-echelon SC with 2 manufacturers and 3 DCs which supply 5 products to 6 customers is considered. The distribution lead times between manufacturers and DCs and between DCs and customers are 1 week. The production capacities which include the available machine processing time and labour processing time at manufacturers are allocated to products based on products' demands. This means that the higher the demand for a product, the higher its share of production capacity. The available machine processing time at each manufacturer is 40 h per week. The available workforce in each manufacturer is 10 and each labour works 40 h per week. Tables 5 and 6 report the machine time and labour time required for processing each product at manufacturers. Table 7 presents the demand for each product under no disruption and demand and lead time disruptions scenarios. If a DC cannot fulfil his customers' demands in full using its inventory, the unmet order is backlogged. This negatively impacts the service level of a DC which is the ratio of the DC sales rate to his customers' demands.

We assume that the two SC echelons operate according to a periodic-review inventory policy with a review period of 1 week. This means every week each SC member reviews its inventory and work-in-process (WIP) and

Table 5. Machine processing time for each product at manufacturers.

Manufacturer	Product				
	P1	P2	P3	P4	P5
Manufacturer 1	12.56	6.82	9.76	11.64	8.12
Manufacturer 2	13.47	5.28	9.87	13.23	7.56

Table 6. Labour processing time for each product at manufacturers.

Manufacturer	Product				
	P1	P2	P3	P4	P5
Manufacturer 1	2.56	3.52	5.46	7.24	6.12
Manufacturer 2	3.47	2.28	6.37	6.23	7.36

places an order with its upstream member. The WIP represents the orders that have been sent by the upstream member but still have not been delivered. The sequence of events for each SC member is as follows: (1) receive the products that were ordered the previous week (lead time = 1) and added to the inventory. Storage capacities for SC members are limited. (2) Use the inventory to meet orders received from downstream members and backlogs (if they exist). (3) Send products downstream and update the inventory positions (both net inventory and WIP) and if necessary generate a backlog. (4) Use the order-up-to (OUT) policy developed by Mosekilde, Larsen, and Serman (1991) to calculate the amount to order to the upstream member. The employed OUT policy has been widely used in the literature (e.g. Aslam and Ng 2016; Goodarzi et al. 2017; Priore et al. 2019). The amount to order is calculated using Equation (2). Each member seeks to meet the average demand (\bar{D}) of its downstream member and bridge the gaps between inventory and WIP with their corresponding desired values.

$$OP_t = \text{Max}(0, \bar{D} + \alpha \underbrace{(DI - (\overbrace{INV_t - B_t}^{NI}))}_{INVGAP}) + \underbrace{\beta(DWIP - WIP_t)}_{WIPGAP} \quad (2)$$

The desired inventory and the desired WIP are constant values that are specified by each SC member. α is the inventory proportional controller and β is WIP proportional controller. These proportional controllers give a weight between 0 and 1 to the gap terms (Disney et al.

2007). A high α represents an aggressive policy for bridging the inventory gap and a high β indicates that all pending delivery orders have been considered when deciding on the amount of order to be placed with the upstream member.

We applied the DES methodology to represent the dynamics of the studied SC. The simulation model is developed using the Simply library in python to analyse the impact of demand and lead time disruptions on the SC service level. The simulation time is 52 weeks, one year, with a warm-up period of 12 weeks. The Simulation time step is 1 week. We used the simulation run monitoring and output data analysis to verify the simulation model. To validate the output results of the simulation, 100 replications have been performed to reduce the output randomness. For testing, we compared the results of the replications.

3.1.3. Optimisation model

The following mathematical notations are defined to formulate the optimisation model for addressing the SC master planning problem:

Indices

i	Index of products $i = 1, 2, \dots, P$
j	Index of manufacturers $j = 1, 2, \dots, F$
k	Index of distribution centres $k = 1, 2, \dots, D$
c	Index of customers $c = 1, 2, \dots, C$
t	Index of period $t = 1, 2, \dots, T$

Parameters

c_{ijt}	Production cost per unit of product i in manufacturer j in period t
tc_{ijkt}	Transportation cost per unit of product i from manufacturer j to distribution centre k in period t
tc_{ikct}	Transportation cost per unit of product i from distribution centre k to customer c in period t
hf_{ijt}	Holding cost per unit of product i at manufacturer j in period t
hd_{ikt}	Holding cost per unit of product i at distribution centre k in period t
u_{ikct}	Tardiness cost per unit of product i not delivered from distribution centre k to customer c in period t
k_{ijt}	Cost of one operator processing product i at manufacturer j in period t

Table 7. Demand of products in each scenario.

Scenario	Product				
	P1	P2	P3	P4	P5
No disruption	Uniform (30, 60)	Uniform (15, 30)	Uniform (32, 64)	Uniform (20, 40)	Uniform (25, 50)
Demand and lead time disruption	Uniform (52, 104)	Uniform (26, 52)	Uniform (56, 112)	Uniform (35, 70)	Uniform (43, 86)

ptm_{ijt}	Machine processing time required per unit of product i at manufacturer j in period t
ptw_{ijt}	Labour time required per unit of product i at manufacturer j in period t
d_{ikct}	Demand of customer c from distribution centre k for product i in period t
a_{jt}	Time available per workforce at manufacturer j in period t
w_{jt}^{max}	Maximum number of workforce available at factory j in period t
pc_{jt}	Available machine processing time at manufacturer j in period t
MIM_{it}	Minimum inventory of product i at manufacturers in period t
MID_{it}	Minimum inventory of product i at distribution centres in period t
ICM_j	Maximum inventory capacity at manufacturer j
ICD_k	Maximum inventory capacity at distribution centre k
L	Distribution lead time from factories to distribution centres

Decision variables

Continuous

x_{ijt}	Number of product i to be produced at factory j in period t
y_{ijkt}	Number of product i to be transported from factory j to distribution centre k in period t
z_{ikct}	Number of product i to be transported from distribution centre k to customer c in period t
s_{ijt}	Number of product i held at factory j at the end of period t
q_{ikt}	Number of product i held at distribution centre k at the end of period t
v_{ikct}	Number of product i not delivered from distribution centre k to customer c in period t , i.e. Backlog

Decision variable

Integer

w_{ijt}	Number of operators processing product i at factory j in period t
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The objective function (1) sets the minimisation of SC total cost (TC) that contains production costs for manufacturers, transportation costs between manufacturers and DCs and between DCs and customers, inventory holding costs at manufacturers and DCs, backlog cost and workforce cost.

$$\begin{aligned} \text{Minimise } TC = & \sum_{t=1}^T \sum_{j=1}^F \sum_{i=1}^P x_{ijt} c_{ijt} \\ & + \sum_{t=1}^T \sum_{k=1}^D \sum_{j=1}^F \sum_{i=1}^P y_{ijkt} t_{c_{ijkt}} \end{aligned}$$

$$\begin{aligned} & + \sum_{t=1}^T \sum_{c=1}^C \sum_{k=1}^D \sum_{i=1}^P z_{ikct} t_{c_{ikct}} \\ & + \sum_{t=1}^T \sum_{j=1}^F \sum_{i=1}^P s_{ijt} h_{f_{ijt}} \\ & + \sum_{t=1}^T \sum_{k=1}^D \sum_{i=1}^P q_{ikt} h_{d_{ikt}} \\ & + \sum_{t=1}^T \sum_{c=1}^C \sum_{k=1}^D \sum_{i=1}^P v_{ikct} u_{ikct} \\ & + \sum_{t=1}^T \sum_{j=1}^F \sum_{i=1}^P w_{ijt} k_{ijt} \end{aligned} \quad (3)$$

Constraint (2) gives the available machine processing time upper bound which is 40hrs per week. Constraints (3) states that the inventory level of each product at each factory for each period is equal to the number of products produced minus the number of products that flow out to the distribution centres plus the inventory that is left over from the previous period. Constraint (4) states that the net inventory level of each product at each distribution centre for each period t is equal to the sum of products that are sent by the factories at time $t-L$ and arrive at the distribution centre at time t minus the amount of products that flow out of the distribution centre to customers at time t plus the net inventory that is left over from the previous period, i.e. $t-1$. L represents the distribution lead time from factories to distribution centres.

$$\sum_{i=1}^P ptm_{ijt} x_{ijt} \leq pc_{jt} \quad \forall j, t. \quad (4)$$

$$s_{ijt} = x_{ijt} - \sum_{k=1}^D y_{ijkt} + s_{ijt-1} \quad \forall i, j, t. \quad (5)$$

$$q_{ikt} - v_{ikct} = \sum_{j=1}^F y_{ijkt-L} - \sum_{c=1}^C z_{ikct} + q_{ikt-1} - v_{ikct-1} \quad \forall i, k, t. \quad (6)$$

Constraint (5) enforces the number of products shipped from distribution centres to each customer in each period to be less or equal to the customer's demand in the same period plus the backlog from the previous period. Constraint (6) calculates the backlog of each product by subtracting the number of products that are sent to each customer from customer demand.

$$z_{ikct} \leq d_{ikct} + v_{ikct-1} \quad \forall i, k, c, t. \quad (7)$$

$$v_{ikct} = d_{ikct} - z_{ikct} \quad \forall i, k, c, t. \quad (8)$$

Constraint (7) states the required labour processing time must be less or equal to the available labour processing time. Constraint (8) ensures that the number of workforces is less or equal to the max number of the available workforce. Constraints (9) and (10) ensure that the inventory level for each product is greater or equal to the minimum inventory level of the product. Constraints (11) and (12) enforce that the aggregated inventory of products does not exceed the maximum inventory capacity. Finally, constraint (13) enforces the non-negativity of the decision variables.

$$\sum_{i=1}^P p_{t w_{ijt}} * x_{ijt} \leq a_{jt} * w_{ijt} \quad \forall j, t. \quad (9)$$

$$\sum_{i=1}^P w_{ijt} \leq w_{jt}^{max} \quad \forall j, t. \quad (10)$$

$$MIM_{it} \leq s_{ijt} \quad \forall i, j, t. \quad (11)$$

$$MID_{it} \leq q_{ikt} \quad \forall i, j, t. \quad (12)$$

$$\sum_{i=1}^P s_{ijt} \leq ICM_j \quad \forall j, t. \quad (13)$$

$$\sum_{i=1}^P q_{ikt} \leq ICD_k \quad \forall k, t. \quad (14)$$

$$x_{ijt}, y_{ijkt}, z_{ikct}, s_{ijt}, q_{ikt}, v_{ikct} \geq 0, w_{ijt} \in \mathbb{Z}^+. \quad (15)$$

4. What is the impact of SC disruptions on SC performance?

This section is focused on the first research question, what is the impact of disruptions on SC service level?

Four scenarios are designed to investigate the impact of disruptions on the SC service level.

The global settings for all modelling scenarios are shown in Table 8. As it was shown in Table 7, we use a uniform distribution to represent the demands of all products. The demands of products can also be expressed using alternative distributions, such as Normal and Poisson.

Table 8. Global settings for all disruption scenarios.

Run time	52 weeks
Warm-up period	12 weeks
Inventory proportional controllers (all SC members)	0.5
WIP proportional controllers (all SC members)	0.2
Desired inventories (each product at DCs and manufacturers)	3 times minimum customer demand
Desired WIPs (each product at DCs and manufacturers)	3 times minimum customer demand
Distribution lead time between SC members	1 week
DES model timing of action	1 week

4.1. Scenario 0: no disruption in SC

This scenario serves as a baseline scenario and shows the performance of the SC when no disruption exists. The impacts of disruptive events are compared with the results obtained from a no disruption scenario. Figure 3 shows demand, the mean inventory levels at SC members, and the mean DCs service level for all products. As it can be seen, for all products the mean inventory levels held by the manufacturers is higher than the inventory levels held by the DCs. The reason for this is that the DCs receive customers' demand for each product. While the manufacturers receive the DCs' demand which contains DCs' inventory and WIP gaps in addition to the customers' demands for each product. Under a no disruption scenario the average fill rates for DCs and manufacturers remain at 100% throughout the 52 weeks of simulation.

4.2. Scenario 1. Demand disruption

This scenario studies the impact of an increase in customer demand on SC performance. Figure 4 illustrates the impact of customer demand growth by 75% for all products from week 16 to week 36 on SC performance. This means that the lower and upper bounds of demand for each product increase by 75%. The mean inventory levels of all products at SC members fall during the disruption which results in drops in the service level of the DCs for all products. Table 9 shows the impact of disruption duration on SC performance. The 95% confidence intervals (CIs) for the mean manufacturers' inventory, mean DCs inventory, and mean DCs service level that is calculated from 100 simulation runs are reported. The longer the disruption time, the lower the mean of inventory values at the SC members and the lower the mean of DCs service level. For instance, compared to the no disruption scenario the 20-week demand growth reduced the mean of product 1 inventory at DCs and manufacturers by 71% and 56%, respectively. This also led to a 3% reduction in mean DCs service level for product 1.

4.3. Scenario 2. Lead time disruption

This scenario studies the impact of distribution lead time extension caused by delays at international borders. Figure 5 illustrates the impact of an increase in distribution lead time from manufacturers to DCs and from DCs to customers by 1 week between weeks 16 and 36 on SC performance. The mean inventory levels of all products at DCs fall during the disruption which results in drops in the service level of the DCs for the products. For

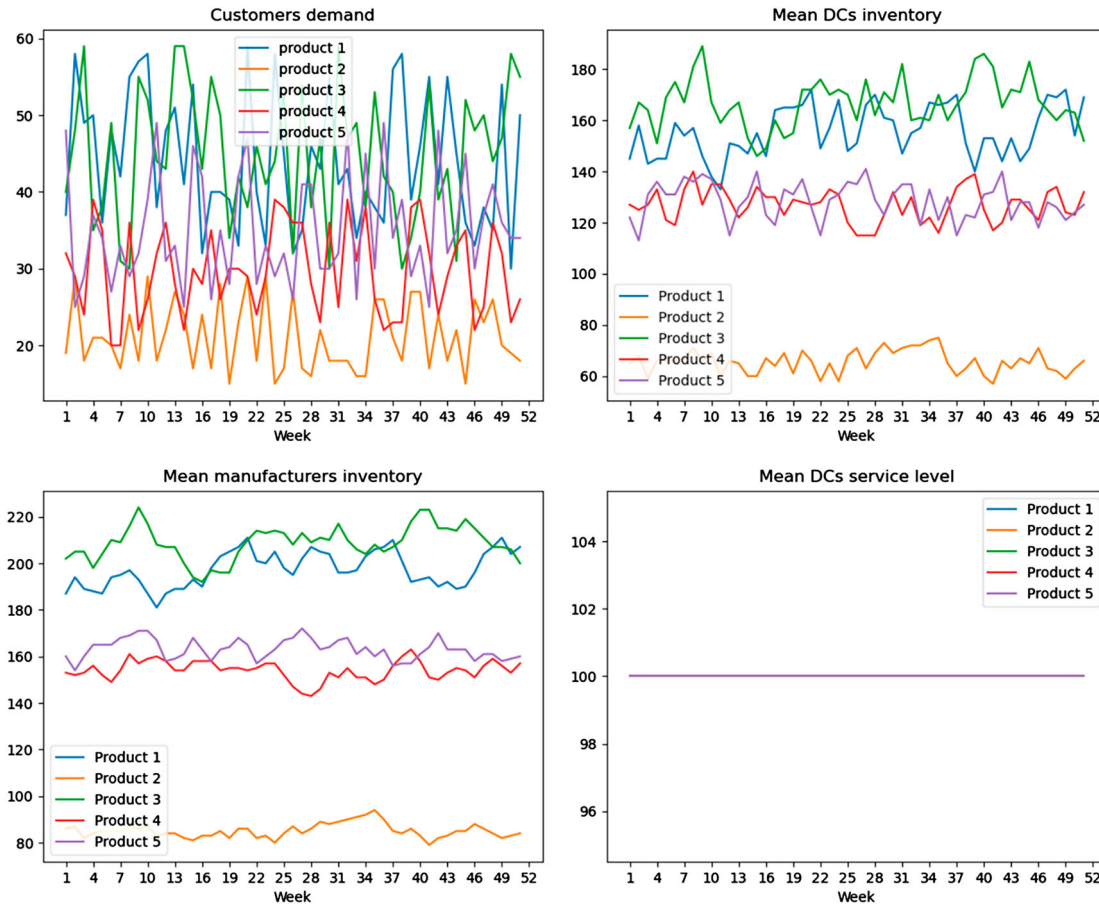


Figure 3. Experiment results: No disruption.

instance, compared to the no disruption scenario the 20-week lead time extension reduced the mean of product 1 inventory at DCs and manufacturers by 43% and 21%, respectively. This also led to a 4% reduction in mean DCs service level for product 1. This shows that the demand increase has a higher impact on reducing inventory levels at SC members than the lead time extension. The reason for the reduced inventory levels at manufacturers is that at the start of the lead time disruption, the week 16 wholesaler increases its demands as they strive to bridge the gap between its desired inventory of products and its actual inventory of products impacted by the disruption. This reduces inventory levels at the manufacturers which results in lower mean inventory levels of the products at the manufacturer compared to the no disruption scenario.

4.4. Scenario 3. Demand and lead time disruptions

This scenario combines scenarios 1.1 and 1.2 to investigate the impact of simultaneous disruptions in demand and lead time on SC performance. In this scenario, demand grows by 75% and lead time from manufacturers to DCs and from DCs to customers increases by 1

week between week 16 and week 36. As Figure 6 shows, the mean inventory levels of all products at manufacturers and DCs fall during the disruption which results in the drops in service level of the DCs for the products. For instance, compared to the no disruption scenario the 20-week demand growth and lead time extension reduced the mean of product 1 inventory at DCs and manufacturers by 78% and 62%, respectively. This also led to an 18% reduction in the mean DCs service level for product 1. This shows that the impact of this scenario, i.e. demand and lead time disruptions, on mean inventory levels at SC members and mean DCs service levels for all products is higher than Scenario 1.1, i.e. demand increase, and scenario 1.2, i.e. lead time extension.

The results of the studied scenarios show that demand and lead time disruptions have adverse impact on SC service level. This adverse impact should be prevented by updating minimum inventory levels held at SC members in line with demand and lead time disruptions. As it is shown in Figure 2, machine learning can identify the new minimum inventory levels held at SC members using the data generated by the simulation model after considering the disruptions. This is elaborated in Section 5.

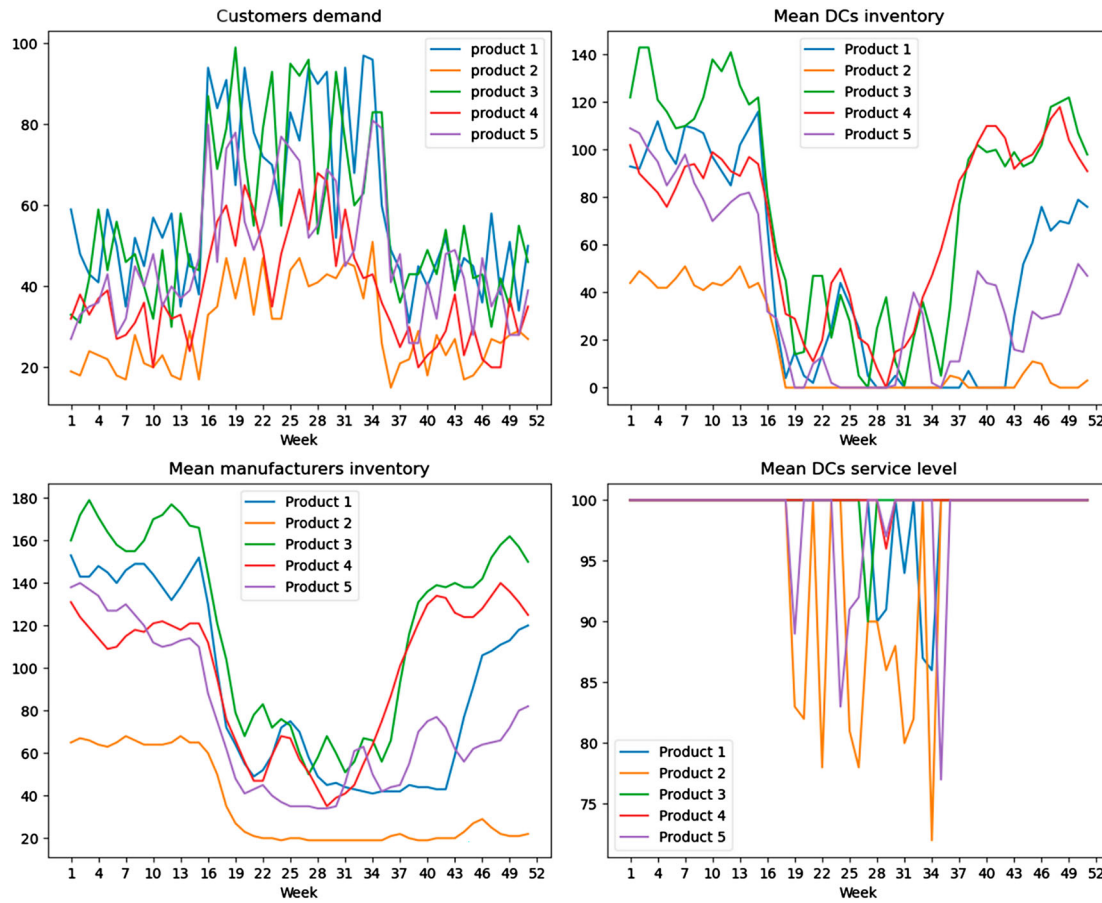


Figure 4. Experiment results: Demand disruption.

Table 9. Impact of demand increase duration on SC performance.

SC Performance		Disruption time (days)			
Indicator 95% CI		5	10	15	20
Mean DCs inventory	P1	[72 ± 4]	[64 ± 7]	[55 ± 10]	[46 ± 12]
	P2	[52 ± 3]	[34 ± 4]	[22 ± 6]	[15 ± 6]
	P3	[95 ± 8]	[87 ± 10]	[82 ± 11]	[78 ± 13]
	P4	[73 ± 5]	[71 ± 5]	[71 ± 7]	[69 ± 10]
	P5	[58 ± 4]	[47 ± 6]	[43 ± 8]	[39 ± 10]
Mean manufacturers inventory	P1	[118 ± 7]	[103 ± 9]	[96 ± 10]	[89 ± 11]
	P2	[79 ± 4]	[62 ± 5]	[47 ± 6]	[35 ± 6]
	P3	[134 ± 7]	[128 ± 9]	[125 ± 10]	[120 ± 12]
	P4	[132 ± 5]	[119 ± 6]	[104 ± 8]	[96 ± 9]
	P5	[144 ± 6]	[115 ± 9]	[91 ± 9]	[75 ± 10]
Mean DCs service level	P1	[98.55 ± 1.42]	[97.80 ± 0.97]	[96.59 ± 0.99]	[97.08 ± 1.72]
	P2	[98.71 ± 0.81]	[98.39 ± 1.14]	[97.82 ± 1.48]	[95.88 ± 1.89]
	P3	[98.55 ± 1.32]	[96.33 ± 1.75]	[95.62 ± 2.33]	[97.37 ± 2.67]
	P4	[100 ± 0]	[99.25 ± 0.28]	[99.11 ± 0.49]	[98.52 ± 0.73]
	P5	[98.58 ± 1.22]	[97.01 ± 1.25]	[94.09 ± 1.80]	[95.35 ± 1.84]

5. How can a hybrid modelling framework maximise SC service level in the presence of disruptions while minimising SC total cost?

This section addresses research question 2, how can a hybrid modelling framework identify an optimal SC master plan to maximise SC service level in the presence of disruptions while minimising SC total cost?

5.1. Insights on inventory management using the decision tree algorithm

As was discussed in Section 3.1.1, the decision tree algorithm needs data in the form of a feature-value table to generate the decision rules. We consider the mean inventory values of a product at manufacturers and DCs as features and the mean DCs service level for the product

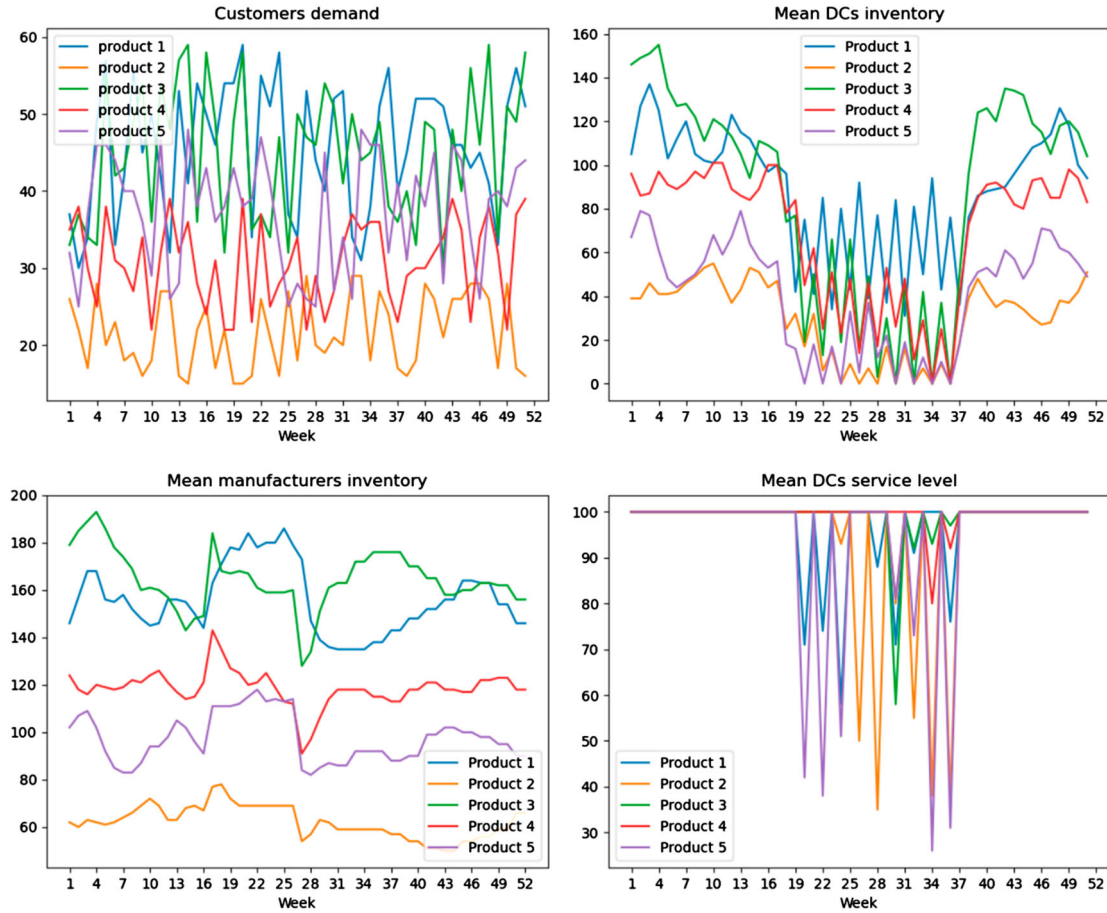


Figure 5. Experiment results: Lead time disruption.

as value. We consider two classes to represent the mean DCs service level of a product: (1) low represents the service level below 98% and (2) high represents the service level above 98%. We follow the procedure presented in Figure 7 to generate data for the decision tree algorithm. Firstly, feasible intervals for inventory replenishment parameters are defined within the simulation model. These include inventory proportional controller (α), WIP proportional controller (β), desired inventory, and desired WIP. The inventory and WIP proportional controllers follow a uniform distribution in the range $[0, 1]$ and the desired inventory and desired WIP follow a uniform distribution in the range $[0, 3 \times \text{max customer demand}]$ in line with prior works in the literature (e.g. Ciancimino et al. 2012; Dominguez, Framinan, and Cannella 2014; Priore et al. 2019). Thereafter, the simulation model is run for 1600 weeks and the mean inventory values of all products at manufacturers and DCs and corresponding classes for the mean DCs service levels for the products are recorded for each week.

We employ the CART algorithm in the Scikit-learn library to structure the inventory management knowledge obtained from the training dataset into a decision

tree. The 10-fold cross-validation method is used to validate the results. This randomly divides the example set into 10 subsets, 9 of which are used for knowledge extraction and 1 is used for testing the decision tree by calculating the number of examples which were classified correctly. This process is repeated ten times and the average of the results known as hit ratio is reported. This metric represents the accuracy of the decision tree algorithm. Figure 8 displays the hit ratio for different sizes of the training dataset (between 100 and 2000 examples). As expected, the hit ratio improves as the number of examples increases. Nonetheless, this indicator stabilises in a narrow range, approx. 89–92%, over 100 examples. The slight variability is mainly caused by the randomness of the examples chosen by the cross-validation method. Overall, it is observed that the decision tree algorithm is capable of capturing the relationships between the inventory levels of the products and DCs service levels for the products.

The design of a decision tree highly impacts its accuracy. The higher the depth of a decision tree, the higher its accuracy. Although, this only applies to training data and the accuracy of a decision tree on test data will not

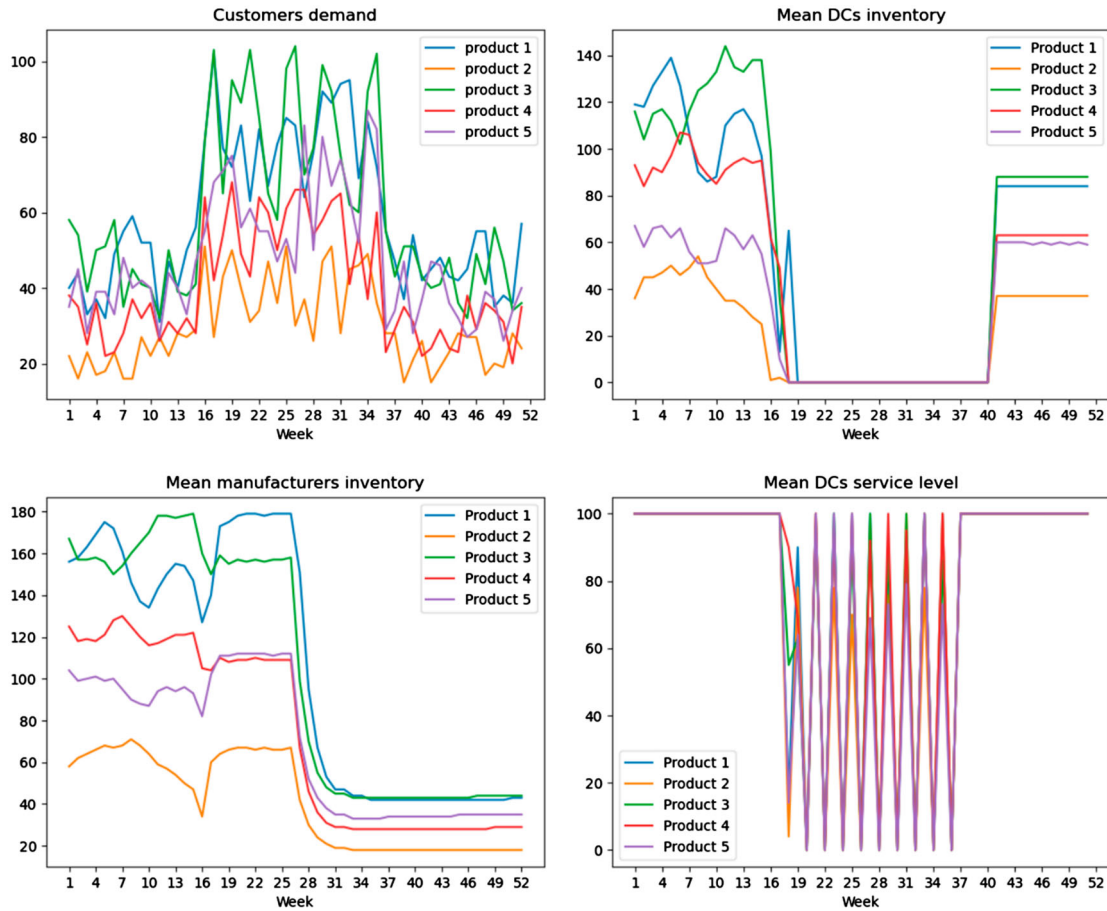


Figure 6. Experiment results: Demand and lead time disruptions.

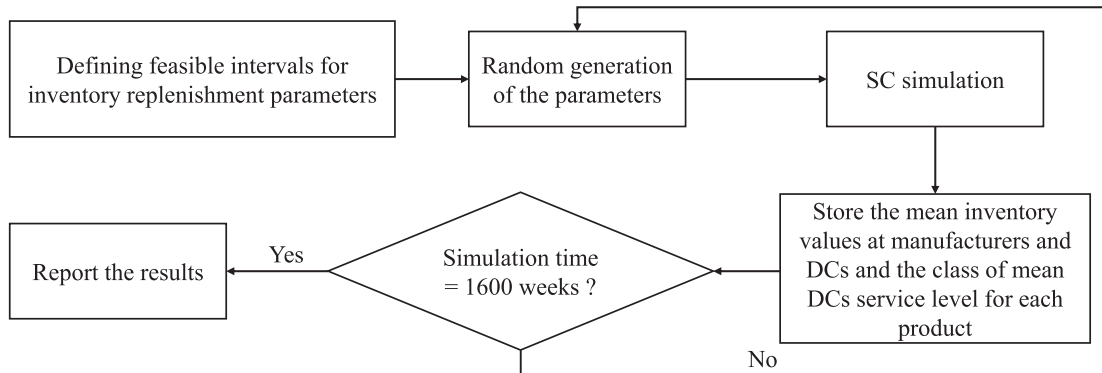


Figure 7. Flow diagram for generating data.

improve beyond a certain depth. If a decision tree grows beyond this certain depth, the tree will overfit the training data which means the decision rules extracted from the tree are unreliable (Priore et al. 2019). To prevent overfitting, the hyperparameters of a decision tree need to be tuned. This is known as pruning. Among the decision tree parameters, the max depth of the tree plays a key role in overfitting prevention. To find the optimal max depth of the decision tree, we follow two steps: (1) creating a full tree without setting any max depth. This results in a

decision tree with depth 8. (2) Using Grid search which is a hyperparameter tuning technique to find the max tree depth that produces the highest accuracy on test data. This is known as the optimal max depth of the tree, and we found it to be 4 in our case. Therefore, we set the max depth of the decision tree to be 4.

Figures 9 and 10 represent the decision tree with max depth 4 for no disruption and demand and lead time disruptions scenarios, respectively. These figures show the branches generated from mean DCs product 1 inventory

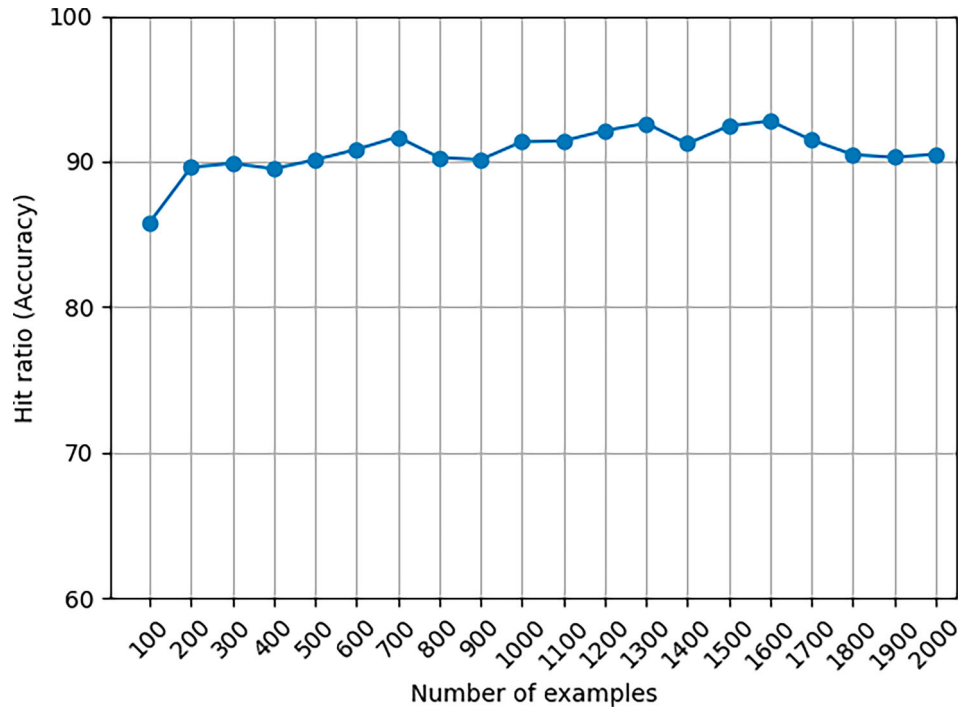


Figure 8. Relationship between accuracy and number of examples in the training dataset.

Table 10. Extract of decision rules.

Rule	If	Then	Hit ratio
1	DC_inventory_p1 > 58	high	989/989
2	55 ≤ DC_inventory_p1 ≤ 58	high	48/51
...			
11	30 < DC_inventory_p1 ≤ 38 and m_inventory_p1 ≤ 93	low	20/25
12	DC_inventory_p1 ≤ 30	low	227/227

and mean manufacturers' product 1 inventory. The class variable at the bottom of each box indicates the class of mean DCs service level. Classes low and high are represented by blue and brown boxes, respectively. Various combinations of the two attributes result in different inventory policies. Under no disruption scenario, 12 decision rules are extracted by the decision tree algorithm from which 8 result in a high mean DCs service level, i.e. more than 98%, and 4 lead to low mean DCs service level, i.e. below 98%. Under the demand and lead time disruptions scenario, the decision tree algorithm generates 13 decision rules from which 9 result in the high mean DCs service level and 4 lead to the low mean DCs service level.

As an illustration, Table 10 reports some of the rules for the no disruption scenario. Next to each rule, the ratio of the number of examples properly classified over the total number of examples that verify the conditions of the rule known as the hit ratio is reported. For instance, rule 11 states that if the mean DCs product 1 inventory is

between 30 and 38 and the mean manufacturers' product 1 inventory is less or equal to 93, the mean DCs service level is predicted to be low which means the mean DCs service level is lower than 98%.

The decision tree illustrates the order of relevance of the features. The features which are higher in the decision tree are more significant in explaining the target, i.e. value. For instance, in the decision tree depicted in Figures 9 and 10, the mean DCs inventory is the most relevant attribute in explaining the mean DCs service level. This was expected as the mean DCs inventory is the determinant factor for the mean service level which is provided by the DCs. It can also be seen in both figures that a high mean DCs service level can be provided through following two policies: (1) holding inventory levels close to the upper interval of the customers' demand at DCs, i.e. rule 1 (2) keeping inventory as high as 2.3 times upper interval of the customers' demands at the manufacturers and holding lower inventory than policy 1 at the DCs, i.e. rule 11. Under the no disruption scenario where the distribution lead time from manufacturers to DCs is stable, implementing policy 2 provides saving opportunities on transportation costs and therefore it is more economical to implement policy 2. While in the presence of demand and lead time disruptions in which the distribution lead time from manufacturers to DCs is extended, deploying policy 2 may compromise the mean service level by the DCs. Moreover, Figures 9

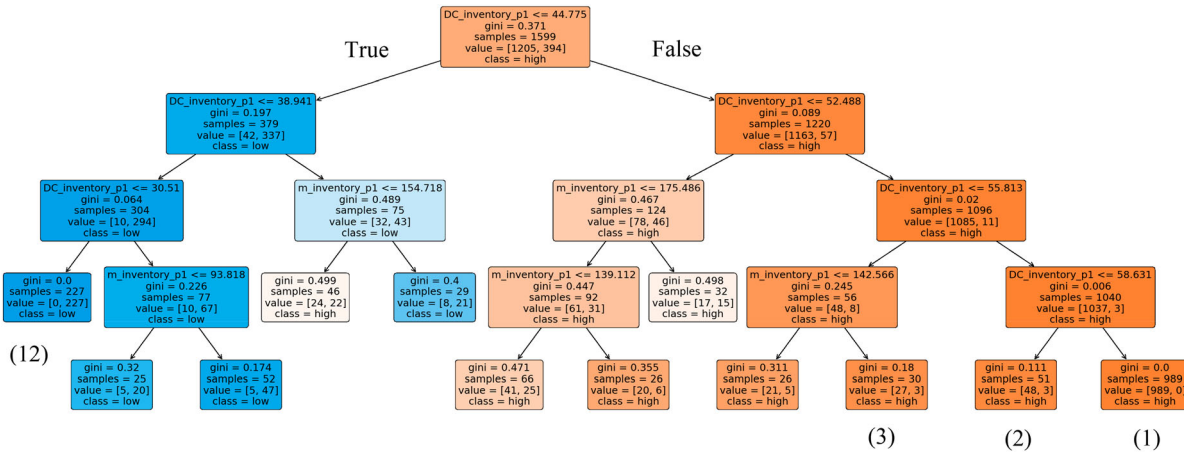


Figure 9. Decision tree for no disruption scenario.

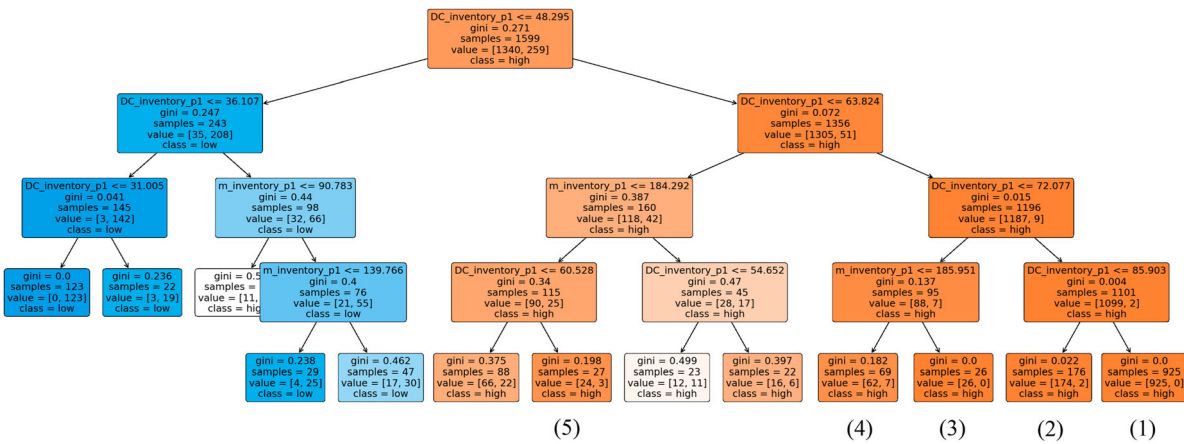


Figure 10. Decision tree for demand and lead time disruptions scenario.

and 10 reveal that DCs and manufacturers need to keep higher inventory under demand and lead time disruptions scenario than in the no disruption scenario to keep a high mean DCs service level. This is in line with the findings by (Ivanov et al. 2019) that recommend increasing inventory throughout the SC as a proactive strategy for dealing with SC disruptions.

5.2. Insights on identifying the optimal SC decisions using optimisation

The developed optimisation model in Section 3.1.3 can determine the optimal production, storage, and distribution decisions in SCs under no disruption and demand and lead time disruption scenarios. The data presented in Tables 4–6 are used to demonstrate the applicability

Table 11. Results from optimisation model for each scenario.

Scenario		Decisions							SC total cost
		$\sum_{j,t} x_{ijt}$	$\sum_{j,k,t} y_{ijk,t}$	$\sum_{k,c,t} z_{c,t}$	$\frac{\sum_{j,t} S_{ijt}}{52 * 2}$	$\frac{\sum_{k,t} q_{ikt}}{52 * 3}$	$\sum v_{ikct}$	$\frac{\sum_j w_{jt}}{52 * 2}$	
No disruption	P1	6539	5499	2483	20	58	0	6	173258
	P2	3059	2279	875	15	27	0	0	
	P3	6915	5719	2547	23	61	0	0	
	P4	4563	3627	1755	18	36	0	0	
	P5	5174	4498	2054	13	47	0	0	
Demand and lead time disruption	P1	8983	8983	3991	0	96	0	10	301227
	P2	4043	4043	1703	0	45	0	0	
	P3	9620	9620	4368	0	101	0	0	
	P4	5993	5993	2769	0	62	0	0	
	P5	7020	7020	2964	0	78	0	0	

Table 12. Impact of lead time on mean inventory values and SC total cost.

Lead time		Decisions		SC total cost
		$\sum_{j,t} s_{ijt}$	$\sum_{k,t} q_{ikt}$	
		52 * 2	52 * 3	
L = 1	P1	27	58	173258
	P2	15	27	
	P3	23	61	
	P4	18	36	
	P5	13	47	
L = 2	P1	21	82	243952
	P2	11	35	
	P3	18	86	
	P4	15	52	
	P5	9	68	
L = 3	P1	0	100	297620
	P2	0	48	
	P3	0	106	
	P4	0	63	
	P5	0	81	

of the optimisation model. We also perform sensitivity analysis on the distribution lead time parameter to analyse the performance of the optimisation model. It should be noted that all numerical experiments are implemented in Pyomo and solved using the CPLEX 20.0 solver on an Intel(R) Core (TM) CPU i7-10610U @2.60 GHz with 32GB RAM. Since the developed model is linear, the solution times in our numerical experiments were not significant (i.e. less than 30 sec).

Table 11 reports the mean results obtained from the optimisation model under no disruption and demand and lead time disruptions scenario. Demand and lead time growth increase the inflow of products within the SC and the mean inventory held by the DCs. Although it reduces the mean inventory held by manufacturers. The reason for this is that the optimisation model aims to avoid missing customer demand by keeping all the inventory at DCs. This is in line with policy 1 which was explained in Section 5.1. Another noteworthy observation is that under no disruption scenario the means of optimal inventory values at DCs are equal to the minimum inventory levels recommended by the decision tree algorithm. Although, under the demand and lead time disruptions scenario the means of optimal inventory values at DCs are higher than the recommended values by the decision tree algorithm. This shows the necessity of integrating optimisation with simulation and machine learning to identify the optimal SC decisions.

Table 12 reports the impact of lead time on average inventory levels at DCs and manufacturers. Lead time extension increases the inventory levels at DCs. While it reduces the inventory levels at the manufacturers. This leads to an increase in SC total cost as the unit inventory holding cost in DCs is higher than in manufacturers.

5.3. Responsive vs. unresponsive SC master planning

In this section, the performance of the supply chain operating in a responsive planning manner is compared with the unresponsive alternative under the demand and lead time disruptions. This enables us to investigate the effectiveness of the proposed hybrid modelling framework presented in Figure 2 in minimising the impact of demand and lead time disruptions on SC service level. In the unresponsive case, the minimum inventory levels to be held at SC members are defined by Equations (9) and (10) in the optimisation model are not adjusted in line with the disruptions. Therefore, the SC master plan is not updated in line with the disruptions. While in the responsive case, the minimum inventory levels to be held at SC members are adjusted in line with the disruptions to keep the mean DCs service level at a high level, i.e. above 98%. Therefore, the SC master plan is updated in line with the disruptions.

In the demand and lead time disruptions scenario, nine decision rules that are represented by brown boxes at the end node of the decision tree in Figure 10 lead to the high mean DCs service level. Four of these decision rules have a Gini impurity greater than 0.2 and are excluded from further analysis. We obtain five SC master plans using the hybrid modelling framework presented in Figure 2. We then use simulation to compare the performance of the five responsive SC master plans against three unresponsive alternatives which are obtained from decision rules with a Gini impurity lower than 0.2 in Figure 9, i.e. decision rules 1, 2, and 3.

Table 13 reports the 95% CIs for the mean of DCs service level for each product obtained from 100 simulation runs for the responsive and unresponsive cases under the demand and lead time disruptions scenario. Each run includes 52 weeks. The responsive approach significantly increases the mean DCs service level compared to the unresponsive approach. For instance, the responsive approach increased the mean DCs service level for product 1 under demand and lead time disruptions scenario by 16.88 percent. Rule 1 of responsive policy which recommends holding inventory levels close to the upper interval of the customers' demands at DCs, provides the highest service level or the lowest backlog, therefore, it results in the lowest SC total cost. Following this rule reduces the SC total cost by 15% compared to the rule 1 of unresponsive approach.

In the responsive case, from rules 1 to 5 shown in Figure 10, the minimum inventory to be held by the DCs decrease which results in a reduced mean DCs service level. Although the rate of the mean DCs service level reduction is significantly lower than that of

inventory abatement. For instance, the minimum inventory of product 1 to be held by the DCs in rule 1 is 85 which is 42% higher than the value in rule 5.

To statistically verify that the responsive policy outperforms the unresponsive policy, we used the t-test technique. We have tested the significance of the difference between the means of the DCs service level for each responsive policy and each unresponsive policy and obtained a p -value much lower than 0.05 in all cases. Thus, we reject the null hypothesis (equality of means in unresponsive and responsive cases).

To sum up, our results show the impact of unresponsiveness to SC disruptions on the SC service level. This is caused by not updating the SC master plan in line with disruptions. We demonstrate that responsive policy offers a promising solution for keeping a high SC service level while minimising SC total cost. To implement responsive policy, minimum inventory levels in the optimisation model need to be updated in line with disruptions. This can be achieved by using decision rules on minimum inventory levels at SC members generated by the decision tree algorithm. To generate the decision rules, the decision tree algorithm requires data on disruptions that are provided by simulation. That is why we need to integrate simulation, optimisation, and machine learning to remain responsive in the presence of SC disruptions.

6. Role of hybrid modelling in SC digital twins for master planning

This section addresses research question 3, how can a hybrid modelling framework support the development of a SC digital twin?

A digital twin for SC master planning enables the continuous cycle of improvement and adjustment of the SC in near real-time (Marmolejo-Saucedo, Hurtado-Hernandez, and Suarez-Valdes 2019). To build a digital twin for SC master planning three main steps need to be taken: (1) Collecting real-time or near real-time data on all processes and resources required to generate a SC master plan from the physical SC environment (2) Pre-processing the collected data and (3) Analysing

the pre-processed data in the digital SC environment to inform decision making (Serrano-Ruiz, Mula, and Poler 2021). The main physical processes for SC master planning are: (1) Inventory planning; (2) Production planning (3) and Distribution planning. To execute these processes, resources including machines, labour and inventory are required. Real-time or near real-time data on these processes and resources may be collected from enterprise resource planning (ERP) systems and by using I4.0 enabling technologies such as industrial IoT, i.e. drawing on available data from the Information Technology (IT) and Operating Technology (OT) systems.

The real-time or near real-time data collected on processes and resources come from multiple sources and are usually characterised by incompleteness and redundancy. To address these, data pre-processing is required before the actual use of the collected data. Data pre-processing transforms the collected raw data into understandable and usable forms for analysis. The data pre-processing includes data integration and data cleaning. The data integration combines data that come from multiple sources into a coherent data store. The data cleaning deals with incompleteness and redundancy through estimating missing values and dropping duplicates (Acheme and Vincent 2021).

Simulation, optimisation, and machine learning are the three main techniques for analysing the pre-processed data on SC master planning processes and resources. Each of these techniques has limitations. Simulation and machine learning are not prescriptive and therefore cannot identify the optimal SC decisions. Optimisation would be computationally inefficient if it included the complexities and dynamic behaviour of SCs as simulation and machine learning do. Integrating these three techniques results in overcoming their individual shortcomings and therefore determining the optimal SC master plan in line with disruptions in a reasonable time. The need for such an integrated framework has been highlighted in the studies which presented conceptual frameworks for developing SC digital twins (e.g. Dolgui, Ivanov, and Sokolov 2020; Ivanov

Table 13. 95% CI for the DCs service level for each product under demand and lead time disruptions scenario.

Policy	P1	P2	P3	P4	P5	SC total cost
Unresponsive (rule 1)	[82.06 ± 1.72]	[84.78 ± 1.89]	[85.37 ± 2.67]	[88.52 ± 0.73]	[87.35 ± 1.84]	346549
Unresponsive (rule 2)	[81.92 ± 1.44]	[84.32 ± 1.41]	[85.12 ± 2.15]	[88.16 ± 0.89]	[87.26 ± 1.82]	358221
Unresponsive (rule 3)	[81.65 ± 1.53]	[84.06 ± 1.22]	[84.37 ± 2.35]	[88.05 ± 0.72]	[87.15 ± 1.25]	359533
Responsive (rule 1)	[98.94 ± 0.62]	[99.47 ± 0.43]	[99.32 ± 0.58]	[98.70 ± 0.46]	[98.87 ± 0.51]	301227
Responsive (rule 2)	[98.76 ± 0.73]	[99.32 ± 0.86]	[99.13 ± 0.74]	[98.57 ± 0.52]	[98.64 ± 0.63]	302453
Responsive (rule 3)	[98.51 ± 0.75]	[99.06 ± 0.91]	[98.96 ± 0.83]	[98.46 ± 0.64]	[98.55 ± 0.48]	307621
Responsive (rule 4)	[98.34 ± 0.21]	[98.84 ± 0.75]	[98.56 ± 0.42]	[98.35 ± 0.31]	[98.38 ± 0.57]	310250
Responsive (rule 5)	[98.11 ± 0.16]	[98.36 ± 0.45]	[98.14 ± 0.22]	[98.20 ± 0.62]	[98.15 ± 0.36]	314584
Increase (%)	16.88	14.69	13.95	10.18	11.52	(15)

and Dolgui 2021). Although, the application of such an integrated framework in practice is absent from the literature.

Given this, as shown in Figure 2, we integrate simulation, optimisation, and machine learning techniques in a hybrid framework to identify the optimal master plan in a SC in the presence of disruptions. Without this integration, the use of SC digital twins with real-time or near real-time data would not be effective as the SC master plan could not be adjusted in a reasonable time in line with disruptions. This work therefore provides the essential foundation framework to analyse the collected data on SC master planning processes and resources and make necessary adjustments to cope with disruptions. This framework can be enhanced into a digital twin for SC master planning by upgrading the data flows to real-time or near real-time data on customer demand, distribution lead time between SC members, and available workforce time and machine time at SC members.

7. Concluding discussion

SC disruptions create imbalances in flows of products into the SCs. The COVID-19 pandemic is a recent example of a SC disruption that caused an unprecedented increase in demand and challenged SCs around the globe. There was an unprecedented increase in demand of many products and distribution lead time between SC members extended due to delays at international borders. These have caused unpredictability in inventory levels and shortages at some SC members that consequently reduced service levels to the customers (Ivanov and Das 2020).

This work develops a hybrid modelling framework to determine the optimal production, storage, and distribution decisions under SC disruptions. The developed framework answers three research questions: (1) What is the impact of SC disruptions on SC service level? (2) How can a hybrid modelling framework maximise SC service level in the presence of disruptions while minimising SC total cost? and (3) How can a hybrid modelling framework support the development of a SC digital twin? To answer the first question, the framework uses discrete-event simulation (DES) which is a widely used tool for examining the impact of disruptions on SC performance. To answer the second question, the framework firstly employs the decision tree algorithm which generates decision rules to update the minimum inventory levels of products at SC members in line with disruptions and then applies optimisation to identify the SC master plan. To answer the third question, the role of the developed framework in a SC digital twin is discussed.

7.1. Theoretical and methodology contributions

The use of hybrid modelling for addressing SC planning problems has become increasingly popular among researchers and industry professionals alike (Mustafee et al. 2017). Much of the developed hybrid models in the literature combine two of simulation, optimisation, and machine learning techniques to address SC planning problems. There is a scarcity of studies that show the application of an integrated simulation-optimisation-machine learning framework to address SC planning problems. Although the applications of such frameworks in other domains have been presented (e.g. Dong et al. 2022; Harper and Mustafee 2019; Hou et al. 2022; Mohammadi, Safari, and Vazifekhhah 2022).

This study presented a hybrid modelling framework which integrates simulation, optimisation, and machine learning to address a SC master planning problem in the presence of SC disruptions that overcomes the methodological constraints that exist in each of these techniques and hence work to date. The presented framework uses simulation to incorporate the dynamic behaviour of SCs under demand and lead time disruptions. It uses machine learning to provide explainable solutions with decision rules to determine the optimal SC master plan with minimum inventory values that ensure a service level above 98% for all products. In combination, it uses optimisation to identify the optimal production, storage, and distribution values that minimise the SC total cost. Using this framework, the impact of three SC disruption scenarios were examined, (1) demand increase, (2) lead time extension, and (3) simultaneous demand increase and lead time extension, on the SC service level.

The results showed that under these disruptions, SC service levels for all products dropped because of insufficient inventory levels at DCs. We have also obtained insights on the impact of minimum inventory levels of the products at SC members on SC service levels for the products. Our results show that in the presence of demand and lead time disruptions higher inventory levels should be kept at closest SC members to customers, in this study DCs, than in upstream SC members, manufacturers, to provide the highest service levels for customers. This reduces the level of risk mitigation inventory at upstream SC members (Lücker, Chopra, and Seifert 2021). We show that a service level above 98% can be achieved by maintaining higher inventory levels at manufacturers compared to the DCs. However, this approach comes at the cost of incurring higher SC total cost. Saputro, Figueira, and Almada-Lobo (2021) state that inventory control is not an effective strategy to address long disruptions, i.e. disruptions which last more than 5 days. While we show that our hybrid modelling framework can

effectively tackle long disruptions. As shown in Figure 2, the crucial aspect lies in updating simulation model in line with disruptions and generating new set of data for machine learning model which is responsible for generating decision rules for setting inventory decisions.

SCs can improve their resilience against disruptions by leveraging adaptive strategies (Zhao, Zuo, and Blackhurst 2019). We show that responsive planning in which the minimum inventory levels for the products at the DCs and manufacturers are updated in line with the SC disruptions to keep the mean DCs service level at the high level, i.e. above 98%, is an effective strategy for dealing with disruptions in the SCs. In particular, we show that responsive planning provides a considerably higher service levels for all products and lower SC total cost compared to unresponsive planning. This is in line with the findings by Kamalahmadi, Shekarian, and Parast (2022). We observed that in the responsive case the rate of the mean DCs service level reduction is significantly lower than that of inventory abatement at downstream SC members and inventory growth at upstream SC members. For instance, as shown in Figure 10, the minimum inventory of product 1 to be held by the DCs in rule 1 is 42% higher than the value in rule 5. While service level of rule 5 is 0.83% lower than that of rule 1.

The integrated simulation-optimisation-machine learning framework is one of the main precursors to a SC digital twin. Such a framework is needed to show the data exchange mechanism between modelling techniques before incorporating real-time or near real-time data can be attempted. Rushing into using live data without specifying the data exchange mechanism between modelling techniques will mean that whilst real-time or near real-time modelling can be conducted it is insufficient to address SC master planning problem under disruptions in a reasonable time.

The main limitation of the presented simulation-optimisation-machine learning framework is that scaling it to handle large-scale and real-time scenarios can pose challenges in terms of computational infrastructure requirements. Therefore, it is crucial to guarantee access to an adequate computational infrastructure before attempting to scale such a hybrid framework for large-scale and real-time scenarios.

7.2. Managerial implications

The first step for practitioners wishing to minimise the impact of SC disruptions on SC service level using the presented hybrid modelling framework would be to replicate the known real-world SC in a controllable environment, e.g. through a simulation model. This process includes considering SC disruptions and studying their

impacts on the SC service level. The simulation model enables the exploration of a wide range of scenarios and investigates the suitability of various inventory policies in each scenario.

Secondly, the generated data by the simulation model can be translated into knowledge by a machine learning algorithm, which could establish a set of decision rules for setting minimum required inventory for each product to ensure a high service level to customers in the presence of SC disruptions. This creation of decision rules or policy settings will allow practitioners to not only have a tool to explore disruptions, as in the paragraph above but also to gain insight into varied inventory policies which ensure a high service level.

Thirdly, practitioners aim to minimise SC total cost in addition to keeping a high service level. This is achieved by formulating an optimisation model which helps practitioners to identify optimal production, storage, and distribution decisions which minimise the SC total cost while keeping a high service level. The decision rules from the previous step inform the constraints on inventory levels at SC members.

Fourthly, we have illustrated this process in a case study. The decision tree algorithm has proven to successfully identify the inventory policies that provide a high service level using the data generated by the simulation model. The optimisation model has proven to determine the optimal SC master plan that minimises SC total cost while keeping a high service level. This demonstrates that practitioners can achieve tangible performance improvements using the developed framework.

Finally, the presented hybrid modelling framework also demonstrates the superiority of responsive planning over unresponsive planning in the presence of disruptions to practitioners. We show that responsive planning significantly increases service levels to customers under SC disruptions. Overall, these outcomes illustrate the potential for how the practice could derive better policy settings to achieve higher performance in companies by reaping the benefits of integrated modelling.

7.3. Limitations and future research

To consider directions for future research, the limitations of this work are discussed as follows. Firstly, this study illustrates the application of hybrid modelling frameworks in SC master planning. This framework can be enhanced into a SC digital twin by incorporating real-time or near real-time data on the product and order flows. For instance, real-time or near real-time data on customer demand, distribution lead time between SC members, and available workforce time and machine time at SC members. Secondly, in this paper,

a multi-product forward SC is studied. Future research may consider closed loop SCs. Thirdly, the objective of this work is to minimise SC total cost, while maximising SC service level. Future work can consider other objectives such as minimising carbon emissions. Fourthly, we used the decision tree algorithm to identify the inventory policies which maximise SC service level. Future research may compare the performance of the other machine learning techniques with the performance of the decision tree algorithm in maximising the SC service level. Fifthly, this study only investigates the impacts of disruptions in physical flow on the SC service level. Future research may study the impact of disruptions in information and financial flows in addition to disruptions in physical flow on SC performance. Sixthly, we use a uniform distribution to represent the demands of all products. Future research may utilise alternative distributions such as Normal and Poisson to express the demands of products. A seventh area of research that could develop from the work here is to consider how not just different modelling systems come together but how also different levels of fidelity and scope are brought together. This would contribute to effective modelling at scale. Finally, this study integrated simulation, optimisation, and machine learning to address a SC master planning problem under SC disruptions. Future research could employ the same integrated framework for addressing other SC problems in the presence of disruptions such as supplier selection and network design problems.

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Data availability statement

The data that support the findings of this study are available from the corresponding author, Ehsan Badakhshan, upon reasonable request.

Notes on contributor



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