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Optimization and Simulation for Sustainable Supply Chain Design

Lucas Schreiber

1– Fraunhofer Institute for Material Flow and Logistics

Purpose: This paper provides an overview of analytical optimization models and simulation-based approaches coping with upcoming challenges concerning the growing requirements within the field of sustainable supply chain design. It aims to combine the two highlighted solution methods in order to propose a holistic approach for decision-making support in this area.

Methodology: Initially, a literature review on current application solutions for sustainable supply chain design is given. The regarded and analyzed approaches will be clustered and allocated to supply chain design tasks. Synergetic effects of combining simulation and optimization are identified and an integrated approach is outlined.

Findings: Sustainable supply chain design tasks can be encapsulated in specific modules which are optimized simultaneously. Partial solutions are created which simplify the simulation model and reduce the necessary configurations to verify the robustness.

Originality: Current approaches focusing on sustainable supply chain design mainly use simulation or optimization. A well-defined approach using various preceding optimizations for modularized strategic tasks like partner selection, allocation of resources or determination of transport relations with subsequent verification of the results in a simulation has not been proposed yet.

Keywords: Supply Chain Design, Optimization, Simulation, Sustainability

1 Introduction

The integration of ecological targets within the orchestration of supply chains has been focused increasingly in the most recent research work concerning supply chain management. The strategic orientation of logistics networks, the supply chain design (SCD), represents the most important challenge regarding this topic. It consists of several individual design tasks which influence each other mutually. In current research work, there is only a rudimentary consideration of these interdependencies, since individual planning approaches for the design tasks are integrated isolated from one another (Parlings, et al., 2015). The complexity of supply chain design derives from the task of simultaneously handling the individual design tasks in the best possible way and to identify and to consider the resulting interdependencies. In a best case scenario these interdependencies can be used synergistically.

Supply chain design determines the long-term operational framework and therefore can make the most influential contribution to the establishment of sustainable processes (Krieger and Sackmann, 2018). The drivers of this progressive integration of a sustainable approach include governmental regulations, economic constraints and a growing mentality to save costs caused by rising energy prices (Bonsón and Bednárová, 2015). The last aspect already implies that economic and ecological targets do not necessarily have to be mutually exclusive. On the one hand, resource savings (energy, materials, water, etc.) have a direct positive impact on economic aspects. On the other hand, a conflict of objectives can be identified. If the ecological component exerts a stronger influence on strategic design, for instance, the aim is to bundle transports optimally and to minimize express
transports. This procedure can have an extremely negative effect on the achieved service level (Bretzke, 2014).

This contribution aims to outline a solution framework that realizes a holistic strategy improvement for sustainable supply chain design (SSCD). In the course of this, the interdependencies of the design tasks must be taken into account. In terms of sustainability, it is necessary to include ecological targets within the design tasks on the basis of a uniform system of indicators. The partly negative correlation of the target values should enable the user to create trade-off solutions and compare them with his target preferences. As tools of the solution framework to be outlined, mathematical optimization methods and simulation are used. The analytical mathematical methods are particularly suitable for modeling and coping with the specific design tasks (Seidel, 2009). The simulation represents an efficient tool for the detailed evaluation of the occurring interdependencies in a supply chain. However, one major downside of simulation methods is the high modeling effort (Kuhn, et al., 2010). The linking of optimization and simulation can reduce the modeling complexity of the simulation model by generating initial solutions for individual design tasks using several optimization models beforehand. The subsequent simulation is used to evaluate the dynamic behavior of the supply chain and thus to validate the results (März and Krug, 2011). The results can be implemented into a feedback loop to improve the parameterization of the analytical methods to approximate the specific target preferences.
2 State of the Art Review

This section provides an overview of previous approaches coping with supply chain design tasks using sustainable components. In the following, the drilldown reporting procedure is described. The identified optimization-based approaches are assigned to the individual design tasks. It is quite possible that one approach addresses several design tasks at the same time. In order to realize this assignment it is initially necessary to identify these design tasks. In addition, common approaches for the integration of sustainable components into the supply chain design will be demonstrated. Finally, there is a categorization of the optimization-based solution approaches referring to the type of integration of the sustainable component and the design tasks addressed. Furthermore, simulation-based approaches and combined approaches are introduced and analyzed.

2.1 Supply Chain Design Tasks

The reference model for identifying and classifying the design tasks is the supply chain design task model introduced by Parlings, et al. (2013). It is divided into higher-level supply chain design tasks, supply chain structure tasks and supply chain process design tasks (see Figure 1).
The higher-level tasks represent the definition of a strategy (Basu and Wright, 2017) and the definition of a target system (Schuh and Ünlü, 2012). Since this scope of tasks cannot be sufficiently mathematically or simulative modeled and evaluated, approaches to solutions for these superordinate task are to be excluded in this paper. The structure of the supply chain is developed on the basis of five fundamental design tasks. The first task concerning this scope is the make-or-buy decision. First of all, it must
be determined, which of the offered services are to be provided by the company itself and which are to be purchased from other companies externally (Govil and Proth, 2001).

For services that are not provided by the customer, a partner selection (PS) has to take place. Among other choices, it must be decided whether services are to be sourced regionally or globally and whether a good is to be sourced from just one supplier or several suppliers (Rennemann, 2007). In course of a facility selection (FS), for internal services, such as production, storage or handling of (semi-finished) products, it must be clarified how many different locations are required and where they are located. Inseparable from the choice of location is the task of allocating (A) specific products and the associated resources to the selected locations. Based on the results of the facility selection and allocation, it is necessary to implement an optimal capacity dimensioning (C). For example, production areas, stock areas or production capacities have to be dimensioned (Chopra and Meindl, 2007).

The design of the supply chain structure significantly determines the energy efficiency of the network. However, the make-or-buy decisions only indirectly influence energy efficiency in supply chains, since the definition on the use of internal or external services merely determines the division of processes among the network partners. Therefore, make-or-buy decisions are not considered in detail in this paper.

The third scope of tasks within the supply chain design is the supply chain process design. In the context of the sourcing process design (SPD), concepts for the handling and provision of incoming goods must be established. For example, the implementation of supplier concepts such as "Just-In-Time" or the introduction of a "Vendor-Managed-Inventory" can
be considered in this context. The cooperative agreement with suppliers on strategical optimal delivery rates can also be assigned to this design task.

On the one hand, the production logistics process design (PLPD) consists of the decision concerning the superordinate production strategy (Wilke, 2012). A distinction, for example, can be made between the production strategies make-to-order and make-to-stock. On the other hand, the determination of the order penetration point is also one of the essential decisions within this scope of tasks (Parlings, et al., 2013). When designing the distribution processes (DPD), the most important component is to determine the number of distribution levels for each product. Following the design of sourcing, production and distribution processes, the overarching task of designing the network processes is the development of a suitable replenishment policy for each product, which defines the desired readiness to deliver (Simchi-Levi, et al., 2011).

The design of information and communication processes represents a cross-sectional task that must be addressed from sourcing through production to distribution. The design of the transport relations determines the means of transport to be used for the distribution channels.

The supply chain process design has a significant influence not only on the energy requirements of the individual processes, but also on the efficiency of the service provision. Accordingly, the introduced design task – except for the design of the information and communication processes – are central to the assessment of the energy efficiency of the network and are considered comprehensively in this paper.
2.2 Sustainable Supply Chain Design

The dynamics of supply chains are constantly changing and new paradigms in the context of ecological and social requirements must be anchored in the design of strategic processes (Paksoy, et al., 2019a). Thus, the classic supply chain design can be extended by the factor of sustainability. The aspect of sustainability is understood to mean the potential to minimize risks associated with the scarcity of natural resources, rising energy costs, environmental pollution and waste management (Srivastava, 2007). These potentials are to be integrated as additional indicators into the target system of companies within the framework of supply chain design. This leads to a paradigm shift towards sustainable supply chain design. The newly emerging target values can still be linked with the specific design tasks of classic supply chain design shown in the previous section. In the following, existing optimization models and simulation models for decision support with regard to a sustainable supply chain design will be identified and classified.

2.2.1 Optimization Models for Sustainable Supply Chain Design

In this section, optimization models for the decision support concerning sustainable supply chain design are clustered. Linear, integer linear and nonlinear optimization models are considered. The solution methods used can represent both exact and heuristic methods. The objective function and the constraints of the optimization models should be particularly focused. Since sustainable supply chain design does not necessarily have to optimize monetary values or values that can be projected to a monetary level through an intermediate step, it has to be investigated to what extent
economic and ecological criteria can be included simultaneously. According to Engel, et al. (2009), a general distinction is to be made between four different modeling alternatives (see Figure 2). The first alternative is the direct projection of ecological factors to monetary values. One possibility in terms of energy efficiency is to integrate the resulting energy costs directly into the target function. Likewise, emitted greenhouse gases can be linked to a monetary value within the scope of the emission trading scheme and can accordingly be embedded into a cost-based target function on the basis of the current price for an emission allowance. The second alternative is a weighting of individual subgoals in a higher-level objective function. For this purpose, individual scaling factors for economic and ecological sub-objectives are defined. However, when utilizing weighting factors the determination of the specific scaling factors is problematic (Rösler, 2003). A third form of integration is the establishment of ecological constraints. The consequence is that certain minimum requirements for sustainable components must always be met and that monetary values can only be optimized if the implemented constraints are maintained.
A fourth alternative is the use of multi-objective optimization, also called Pareto optimization. As already shown, optimizations within the framework of sustainable supply chain design are characterized by contradictory target values with regard to several aspects, which influence each other negatively. A resulting challenge is to extract the most efficient trade-off solution, which tolerates losses in one or more target values (Ehrgott, 2005).

The goal of multi-objective optimization is to generate a set of Pareto optimal solutions. In a Pareto efficient state, it is no longer possible to improve a target value without having to worsen another target value. The set of Pareto efficient solutions can then be used to extract a most suitable final solution based on the individual target preferences of the decision-makers (Habenicht, et al., 2003).

In the following step, existing optimization models which provide assistance regarding a sustainable supply chain design are to be clustered with regard to the four modeling alternatives introduced. Within one optimization model, several of the shown modeling alternatives can be used. For example, a multi-objective optimization with sustainable constraints may be provided or a multi-objective optimization can be used to identify suitable
weighting factors, which have to be validated afterwards. The classification regarding the modeling alternative of the respective optimization model is provided in the column "OPT" of Table 1 with the numbering according to Figure 2.

In addition, the classification concerning to the extracted supply chain design tasks (see Figure 1) is provided in Table 1. An optimization model, which manages all tasks simultaneously, could not be identified. The cause for this is the high complexity of the superordinate strategic task and the numerous interdependencies of the individual decisions, which can no longer be handled simultaneously above a certain level of abstraction. Furthermore, a holistic modeling approach would cause an immense calculation effort for decision making over several periods (Günther, 2005). Nevertheless, the models often address more than one design tasks at once, whose scopes have intersections, so that a common integration makes sense up to a certain level. Accordingly, the review includes optimization models, which address at least one strategic design task and also integrate sustainable target values into the objective function in one of the modeling alternatives presented (see Table 1).
Table 1: Optimization models for sustainable supply chain design (own Figure)

<table>
<thead>
<tr>
<th>Source</th>
<th>PS</th>
<th>FS</th>
<th>A</th>
<th>C</th>
<th>SPD</th>
<th>PLPD</th>
<th>DPD</th>
<th>TR</th>
<th>OPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abdallah, et al. (2012)</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td>X</td>
<td></td>
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<td>1,4</td>
</tr>
<tr>
<td>Arslan and Turkay (2013)</td>
<td></td>
<td></td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
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<td>1,3</td>
</tr>
<tr>
<td>Azadnia, et al. (2015)</td>
<td>X</td>
<td></td>
<td></td>
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<td></td>
<td></td>
<td>2,4</td>
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<tr>
<td>Chaabane (2011)</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td></td>
<td></td>
<td>X</td>
<td></td>
<td>3,4</td>
</tr>
<tr>
<td>Guillén-Gosálbez and Grossmann (2009)</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td></td>
<td></td>
<td></td>
<td>4</td>
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<tr>
<td>Jaber, et al. (2013)</td>
<td>X</td>
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<td>1</td>
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<tr>
<td>Lee, et al. (2018)</td>
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<tr>
<td>Source</td>
<td>PS</td>
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<tr>
<td>Mohammadi, et al. (2014)</td>
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<td>X</td>
<td>X</td>
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<td>4</td>
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<tr>
<td>Musavi and Bozorgi-Amiri (2017)</td>
<td>X</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td>4</td>
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<tr>
<td>Paksoy, et al. (2019b)</td>
<td>X</td>
<td>X</td>
<td>X</td>
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<td>2,3,4</td>
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<td>Priyan (2019)</td>
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<td>X</td>
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<tr>
<td>Torğul and Paksoy (2019)</td>
<td>X</td>
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<td>2,3,4</td>
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<tr>
<td>Tsao, et al. (2018)</td>
<td>X</td>
<td>X</td>
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<td>3,4</td>
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<tr>
<td>Yu and Su (2017)</td>
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<td>X</td>
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</table>
In the course of the state of the art review, three different branches with different scopes of application have been identified. The first branch to be mentioned is an analytically sound initial partner selection with integrated sourcing process design under the inclusion of sustainable criteria. The methods are mostly based on fuzzy logic linked to a subsequent linear optimization. There is a variety of configuration options available. Torğul and Paksoy (2019) propose a combination of a fuzzy-based analytical hierarchy process (FAHP) and fuzzy TOPSIS with a subsequent multi-objective linear optimization. Yu and Su (2017) use fuzzy logic linked with a data envelopment analysis (Fuzzy-DEA) and Azadnia, et al. (2015) implement the fuzzy logic in the context of a linear optimization with simultaneous order quantity calculation for the orchestration of partner selection and strategic sourcing process design.

As a second branch, the determination of the network processes based on the lot size determination is to be mentioned. This task includes the design of sourcing, production and distribution processes. As an approach, Arslan and Turkay (2013) propose the extension of the classical economic order quantity (EOQ) calculation to a sustainable economic order quantity (SEOQ). Various possibilities for the inclusion of sustainable components using linear optimization models with ecological constraints are proposed in this context. Priyan (2019) developed an extended nonlinear optimization model as a solution alternative and Jaber, et al. (2013), using another model, calculate optimal production rates in a supplier-producer relationship.

The third and largest branch is concerned with linking the nodes and edges of a supply chain network. In mathematical modeling, the decision varia-
variables represent the transport quantities of the individual products, semi-finished products and raw materials on the edges of the network. In this context the goods are allocated to the locations in the network (see Lee, et al., 2018). The design of the transport relations can theoretically take place in the same step by providing the decision variables a further index as a degree of freedom to determine the means of transport on an edge (see Chaabane, 2011). The distance bridging of the respective edge, the loading weight and the means of transport are factors which have a strong influence on the ecological balance of the network. In addition, binary activation and deactivation variables can be integrated for locations in the network in order to address the design task of facility selection (see Guillén-Gosálbez and Grossmann, 2009). This decision can be extended by a capacity-related degree of freedom so that the decision to use a node in the network has to be made considering different available capacity dimensions (see Paksoy, et al., 2019b; Abdallah, et al., 2012). If the amount of nodes in the network consists of warehouse locations on the distribution side – such as central and regional warehouses – the distribution chain of a product is also determined by this optimization (see Tsao, et al., 2018). In addition, hub allocation problems can be listed especially for the design of strategic distribution processes, which determine optimal links between transshipment points (see Mohammadi, et al., 2014; Musavi and Bozorgi-Amiri, 2017).

### 2.2.2 Simulation Models for Sustainable Supply Chain Design

Besides the mathematical optimization methods introduced, simulation is a common tool for decision support in the context of sustainable supply chain design. The simulation is characterized by the execution of experiments on the basis of a previously created model of an already existing or
planned system. The simulation executes a performance evaluation of the model and the results are projected onto the real system to support the decision-making process (VDI, 2014). In the context of the simulation of supply chains, the dynamic behaviour of the individual locations and their links is simulated in computer models, taking into account the associated processes. The dynamics, i.e. the temporal behavior of the system, is represented by stochastic components with state changes at discrete points in time. The simulation progress takes place by the occurrence of events. For instance, in the simulation of supply chains, these events represent the arrival of a product in a warehouse or the completion of the loading of a means of transport (Rose and März, 2011).

Accordingly, simulation is particularly suitable for the holistic consideration of the interdependencies of the design tasks concerning sustainable supply chain design. Similar to the optimization models, the simulation models must also focus particularly on the performance evaluation under consideration of sustainable criteria. The evaluation is carried out by means of a key performance indicator system to be defined in advance, which determines the indicators to be evaluated after completion of the experiments. In the following, simulation studies already performed in the context of sustainable supply chain design, will be introduced.

One of the first simulative approaches was developed by Hirsch, et al. (1996), in which economically conventional goals such as service level and delivery time are simulative investigated with regard to their ecological compatibility in order to support the establishment of environmentally friendly value networks.

Reeker, et al. (2011) identified suitable methods for the logistics expenses and performance analysis as well as for the ecological assessment, which
were combined to an integrative evaluation approach based on selected key indicators. The interdependencies of the individual target values within the evaluation approach are shown transparently through a simulation.

Cirullies (2016) expanded the logistics target system to include selected ecological indicators such as resource consumption, emission values and energy consumption. Based on this, a global supply chain was modelled in a simulation software and several experiments with varying order penetration points were analyzed. For evaluation and integration into the extended key performance indicator system, transport parameters and location parameters (distance, load weight, etc., depending on the transport process) were converted into an explicitly comparable sustainability value.

2.2.3 Linking Simulation and Optimization for Sustainable Supply Chain Design

It has been shown that optimization methods are particularly suitable for supporting individual design tasks. However, a holistic evaluation is problematic. The simulation can be used for the integrative evaluation of specific scenarios on the basis of a key performance indicator system and unveils the interdependencies of the target values. On the contrary, the definition of suitable scenarios and the choice of parameters for the economic and ecological control parameters within the supply chain is somewhat difficult. A combination of optimization and simulation in the context of sustainable supply chain design is therefore an appropriate possibility to fully exploit the advantages of both tools. According to März and Krug (2011), a distinction is to be made between four different types of linking (see Figure 3).
A few approaches for sustainable supply chain design, which link simulation and optimization can be found. Longo (2012) developed an approach for the simulation of a network with integrated transport route optimization, which can be matched to the integrative linking type number three in Figure 3. In the system of indicators used for the evaluation, the emission values of the transports were examined among other monetary values. Guerrero, et al. (2018) propose an approach based on multi-objective optimization with subsequent simulation to ensure the statistical significance of Pareto solutions. The proposed system of indicators considers the emission values of transports carried out as well as emission values of the individual locations. The approach is to be assigned to the sequential linking type number one (see Figure 3).

The integration of sustainable components is rather sparse in the identified approaches, since only emission values of transport routes or fixed emission values of locations of the network are taken into account. Moreover, not all relevant design tasks are addressed. In the following, an innovative,
Holistic linking approach for sustainable supply chain design will be proposed.

3 Holistic Framework for Sustainable Supply Chain Design

The basic idea of the approach is to synchronize, adapt and extend the results from the state of the art review in an appropriate way. In the context of the identification of optimization models it could be outlined that the profound selection of several models makes it possible to address all relevant design tasks. The interdependencies can be made visible by a simulation – in particular with regard to the interaction of economic and ecological target values. The framework of the innovative approach is based on a combination and extension of the linking types number one and four (see Figure 3). This adaptation is necessary in order to benefit from the advantages of both linking types. Linking type number one is suitable for decreasing the complexity of the subsequent simulation, since initial solutions can already be used, for example, by reducing the number of potential suppliers and locations of the network in advance. Linking type number four already offers a kind of feedback mechanism between optimization and simulation. This is immensely important for the integration of sustainable target values in order to assess the dynamics and interdependencies of the interaction of economic and ecological target values within a supply chain. However, since the approach developed in this paper applies several optimization models simultaneously, the simulative evaluation should not be used for individual optimization models only, but as an evaluation for the overall aggregation of the results across all optimization models used.
In a first step, suitable optimization approaches are extracted, which together cover all relevant design tasks. In section 2.2.1, three superordinate branches have already been identified. The selected approaches from the three branches are to be projected onto the existing supply chain and are synchronized with each other so that they each optimize individual components, which can be aggregated without further intermediate steps. The objective functions to be optimized are based on a previously defined system of indicators. For each model the resulting solution is presented to the decision-makers, who carry out an initial comparison of the individual solutions with the company goals for each optimization model, which results in an initial weighting of the target values. However, the results only consider fixed static periods and usually do not reflect any periodically dynamic effects. To address this issue, a simulation of the aggregated results is executed afterwards. Since the interaction of the aggregated optimizations can deliver a changed overall solution due to mutual interdependencies and the time component, a new evaluation is performed based on the system of indicators. This overall evaluation is in turn presented to the decision-makers, who can adapt the weightings of the individual target values in the optimization models within a feedback loop taking into account the revealed causal relations. Subsequently, a new simulation with aggregated evaluation takes place. This process is repeated until the overall result matches the company goals to be achieved. An overview of the developed framework can be seen in Figure 4.
The first optimization deals primarily with the partner selection. The use of an approach based on the fuzzy set theory with subsequent linear optimization has emerged as state of the art method in literature research.

The criteria to be evaluated should be as consistent as possible with the overall sustainable performance indicator system. The benefit is a complexity reduction of the sourcing nodes of the network to be initially considered. If, in addition, a sourcing strategy is integrated into the model concerning the calculation of optimal sourcing lot sizes and reordering cycles, the sourcing design task is covered simultaneously.

In the second initially isolated optimization, the design of the network processes is the main topic. The determination of potentially optimal lot sizes

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Figure 4: Holistic framework for orchestrating sustainable supply chain design (own Figure)
and replenishment strategies for sourcing, production and distribution is realized, for example, by calculating a sustainable economic order quantity with coupled linear optimization. As a further result, order penetration points to be selected for the individual products can emerge.

The third optimization is responsible for connecting the nodes and edges still available for selection. Each product, semi-finished product or raw material is assigned to a sourcing location, a production location or a distribution location. The company's own locations are dimensioned accordingly with regard to the required resources. To realize the allocations, the resulting edges must be described explicitly with regard to the means of transport to be used and the transport quantities. Since this optimization usually exhibits the highest solution and modeling complexity, heuristic methods are primarily suitable as solving methods. The application of artificial intelligence and machine learning can play a decisive role in finding solutions. Methods such as neural networks or multi-agent systems are becoming increasingly popular in this context, as they are characterized by fast processing of large and complex amounts of data and outperform other solution methods in terms of solution quality and convergence speed (Hellingrath and Lechtenberg, 2019).

The three optimizations have to be adapted to the respective network and synchronized in such a way that the results can be integrated into a simulation software without further effort. Feedback loops may include adjustments to individual models. These adjustments could affect the other optimizations so that they have to be customized simultaneously. The proposed framework is not be regarded as fixed and can be extended modularly by further varying modules and objectives.
4 Conclusion

This paper pointed out that many common optimization models and simulation studies already exist in the field of sustainable supply chain design. In addition, it was highlighted that the combination of the two tools has an immense potential concerning this topic. However, previous combined approaches only address individual supply chain design tasks in isolated cases. Therefore, they cannot make any statements about the interdependencies that occur between the tasks with regard to the dynamics of a supply chain. The integration and evaluation of energy efficiency and ecological factors is also insufficiently developed and has no feedback mechanisms. The innovative holistic approach proposed in this paper addresses all relevant supply chain design tasks and guarantees a sufficient integration of ecological parameters in all components based on a superordinate individual key performance indicator system. Selected state of the art methods are modularly linked and synchronized so that occurring interdependencies of the dynamics of a supply chain can be transparently identified and evaluated. In addition, the feedback loops, which can be performed as often as requested, provide a progressively better configuration with regard to the user's preferences.

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