Deliverable report

Deliverable no./title:	D5.3 Reverse cycle logistics design and evaluation method
Lead beneficiary:	KLU
Nature of deliverable:	Report
Dissemination level:	PU - Public
Due date:	28.02.2022 M33

Grant Agreement number:	820477
Project acronym:	CREAToR
Project title:	Collection of raw materials, Removal of flAme reTardants and Reuse of secondary raw materials
Funding scheme:	H2020-SC5-2018-2019-2020
Coordinator:	FRAUNHOFER GESELLSCHAFT ZUR FOERDERUNG DER ANGEWANDTEN FORSCHUNG E.V.
Project Website:	www.creatorproject.eu

Version history

Version nr	Reviser	Content
V0		Deliverable template
V1	Moritz Jäger-Roschko (KLU)	First draft
V2	Tom Caris (CLR)	Revision
V3	Irma Mikonsaari, Carolyn Fisher (ICT)	Revision

Partners' contribution to the deliverable

Partner	Short name	Role in the WP	Contribution to the deliverable
Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung	ICT	Coordinator	Final review of the deliverable and submission
Coolrec	CLR	WP2 leader, participant in T 5.3	Revision of the deliverable, participation in workshops, data generation
Treee	REL	Participant in T 5.3	Participation in workshops, data generation
ITRB Group	ITR	WP 7+8 leader, participant in T 5.3	Participation in requirement analysis workshops
Kühne Logistics University	KLU	WP5 leader	Main author
All partners		Participant in T5.3	Discussions on the deliverable

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Abbreviations

ANOVA	Analysis of variance
BOM	Bill of materials
EOL	End-of-life
FTL	Full truck load
GIS	Geographic information system
LTL	Less than truck load

1 INTRODUCTION

The project CREAToR (**CREAToR – COLLECT – PURIFY – REUSE (creatorproject.eu)**) focuses on process development and demonstration to remove hazardous, already banned bromine containing flame-retardants from waste streams using continuous purification technologies: supercritical CO_2 and cost-effective solvent-based processes using natural deep eutectic solvents (NADES) in twin-screw extruders. CREAToR will cover the whole value chain, starting from collecting thermoplastic waste streams from building and construction (B&C) and from waste electrical and electronic equipment (WEEE). The project will implement ways to collect secondary raw materials, identify the presence of hazardous flame retardants, remove these contaminants from the materials and finally reuse the materials. As case studies, they will be reused as valuable secondary raw materials for new B&C insulation panels, for automotive interior application, and for producing 3 D printed parts for aerospace applications, creating a circular economy. To further increase the economic feasibility of the approach an optimised logistic concept and a harmonised material quality classification scheme will be developed and applied.

Recycling industries worldwide are central to the transition towards a circular economy. They allow valuable materials to be retrieved from end-of-life products and packaging. Recycling supply chains can only produce high-quality secondary raw materials and be economical if they are well managed. However, the management of the recycling supply chain is complicated as it requires bringing together many players with different objectives and managing uncertainties regarding the quantity and quality of returned products and materials.[1]

The recycling supply chain includes multiple players from waste collection up to the use of secondary raw materials. Managing the supply chain or optimising a firm's operation is challenging. Software solutions specifically designed for use in the circular economy or the recycling industry or containing the tools necessary for the recycling firms are scarce and expensive[2]. Additionally, the recycling industry is not mature in many aspects and is constantly developing. Recycling supply chain planning is a task that only a few firms currently perform, and they often employ spreadsheet-based solutions. These solutions are frequently limited in their capabilities and flexibility and are time-consuming to run.

The academic literature has developed multiple models of recycling supply chains in the context of closed-loop supply chain management and reverse logistics. Several system dynamics models have been developed to investigate the impact of informal recycling[3], ecological motivation and

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[1] V. Jayaraman, A.D. Ross, and A. Agarwal, 'Role of Information Technology and Collaboration in Reverse Logistics Supply Chains', ed. NA, *International Journal of Logistics Research and Applications* 11, no. 6 (2008): 409–25, https://doi.org/10.1080/13675560701694499;
Leonidas Milios et al., 'Plastic Recycling in the Nordics: A Value Chain Market Analysis', *Waste Management* 76 (June 2018): 180–89, https://doi.org/10.1016/j.wasman.2018.03.034.

[2] Clayton Burger, Matthias Kalverkamp, and Alexandra Pehlken, 'Decision Making and Software Solutions with Regard to Waste Management', *Journal of Cleaner Production* 205 (December 2018): 210–25, https://doi.org/10.1016/j.jclepro.2018.09.093.

[3] Maria Besiou, Patroklos Georgiadis, and Luk N. Van Wassenhove, 'Official Recycling and Scavengers: Symbiotic or Conflicting?', *European Journal of Operational Research* 218, no. 2 (April 2012): 563–76, https://doi.org/10.1016/j.ejor.2011.11.030.

technological innovation[4], alternative collection infrastructure[5], taxes and subsidies[6] and deposits[7] on recycling supply chains. Mathematical modelling is used to investigate various recycling supply chain issues, such as recycling facility location problems[8], supply chain design[9] and optimal return channel configurations[10].

However, these models are not well suited for practitioners, as they are usually designed to answer a specific research question and are not very flexible. System dynamics models tend to be relatively high-level and span long time horizons of several decades that extend the planning horizons of managers. Mathematical models are usually stylised and only capture a few aspects and actors of the recycling supply chain. More flexible modelling solutions and tools exist (e.g., Supply Chain Guru, anyLogistix), but these are primarily designed for manufacturing or retail supply chains. The material flow and the processes in these forward supply chains differ significantly from reverse and recycling supply chains. This report therefore investigates the requirements of recycling industry managers regarding supply

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[4] Chihhao Fan et al., 'Modeling Computer Recycling in Taiwan Using System Dynamics', *Resources, Conservation and Recycling* 128 (January 2018): 167–75, https://doi.org/10.1016/j.resconrec.2016.09.006;
P. Georgiadis and M. Besiou, 'Sustainability in Electrical and Electronic Equipment Closed-Loop Supply Chains: A System Dynamics Approach', *Journal of Cleaner Production*, Sustainability and Supply Chain Management, 16, no. 15 (1 October 2008): 1665–78, https://doi.org/10.1016/j.jclepro.2008.04.019;
P. Georgiadis and M. Besiou, 'Environmental and Economical Sustainability of WEEE Closed-Loop Supply Chains with Recycling: A System Dynamics Analysis', *International Journal of Advanced Manufacturing Technology* 47, no. 5–8 (2010): 475–93, https://doi.org/10.1007/s00170-009-2362-7.

[5] Saeed Rahimpour Golroudbary and Seyed Mojib Zahraee, 'System Dynamics Model for Optimizing the Recycling and Collection of Waste Material in a Closed-Loop Supply Chain', *Simulation Modelling Practice and Theory* 53 (April 2015): 88–102, https://doi.org/10.1016/j.simpat.2015.02.001.

[6] Brahmesh Vinayak Joshi et al., 'Impact of Policy Instruments on Lead-Acid Battery Recycling: A System Dynamics Approach', *Resources, Conservation and Recycling* 169 (June 2021): 105528, https://doi.org/10.1016/j.resconrec.2021.105528.

[7] Fan et al., 'Modeling Computer Recycling in Taiwan Using System Dynamics'; Xin Li et al., 'Game-Based System Dynamics Simulation of Deposit-Refund Scheme for Electric Vehicle Battery Recycling in China', *Resources, Conservation and Recycling* 157 (June 2020): 104788, https://doi.org/10.1016/j.resconrec.2020.104788.

[8] Necati Aras et al., 'Locating Recycling Facilities for IT-Based Electronic Waste in Turkey', *Journal of Cleaner Production*, Decision-support models and tools for helping to make real progress to more sustainable societies, 105 (15 October 2015): 324–36, https://doi.org/10.1016/j.jclepro.2015.02.046; Y.T. Chen, F.T.S. Chan, and S.H. Chung, 'An Integrated Closed-Loop Supply Chain Model with Location Allocation Problem and Product Recycling Decisions', *International Journal of Production Research* 53, no. 10 (19 May 2015): 3120–40, https://doi.org/10.1080/00207543.2014.975849;
Bronisław Gołębiewski et al., 'Modelling of the Location of Vehicle Recycling Facilities: A Case Study in Poland', *Resources, Conservation and Recycling* 80 (1 November 2013): 10–20, https://doi.org/10.1016/j.resconrec.2013.07.005;
Farhad Habibi et al., 'A Multi-Objective Robust Optimization Model for Site-Selection and Capacity Allocation of Municipal Solid Waste Facilities: A Case Study in Tehran', *Journal of Cleaner Production* 166 (November 2017): 816–34, https://doi.org/10.1016/j.jclepro.2017.08.063.

[9] Lipan Feng, Kannan Govindan, and Chunfa Li, 'Strategic Planning: Design and Coordination for Dual-Recycling Channel Reverse Supply Chain Considering Consumer Behavior', *European Journal of Operational Research* 260, no. 2 (July 2017): 601–12, https://doi.org/10.1016/j.ejor.2016.12.050; Moritz Fleischmann et al., 'The Impact of Product Recovery on Logistics Network Design', *Production and Operations Management* 10, no. 2 (5 January 2009): 156–73, https://doi.org/10.1111/j.1937-5956.2001.tb00076.x;
H. Krikke, J. Bloemhof-Ruwaard, and L. N. Van Wassenhove, 'Concurrent Product and Closed-Loop Supply Chain Design with an Application to Refrigerators', *International Journal of Production Research* 41, no. 16 (2003): 3689–3719, https://doi.org/10.1080/0020754031000120087;
Zhitao Xu et al., 'Global Reverse Supply Chain Design for Solid Waste Recycling under Uncertainties and Carbon Emission Constraint', *Waste Management* 64 (June 2017): 358–70, https://doi.org/10.1016/j.wasman.2017.02.024.

[10] R. Canan Savaskan, Shantanu Bhattacharya, and Luk N. van Wassenhove, 'Closed-Loop Supply Chain Models with Product Remanufacturing', *Management Science* 50, no. 2 (2004): 239–52;
R. Canan Savaskan and Luk N. Van Wassenhove, 'Reverse Channel Design: The Case of Competing Retailers', *Management Science* 52, no. 1 (January 2006): 1–14, https://doi.org/10.1287/mnsc.1050.0454.

chain modelling tools, determines which features a tool requires to model a recycling supply chain and suggests a method that allows the modelling of recycling supply chains.

To fulfil these objectives in the CREAToR project, Kuhne Logistics University (KLU) is using a six-step methodological approach (see Figure 1). The result of these steps is the Reverse Cycle Design and Evaluation Method. The method helps managers along the recycling supply chain to optimise their operations. Specifically, the method allows the development of a digital twin of the recycling supply chain. This digital twin can be altered to analyse scenarios relevant to the manager – for example, by incorporating new suppliers or altered treatment methods and answering 'what if?' questions. The method will be further tested and deployed in a specific use case in task 5.4 of the CREAToR project and will be reported later in March 2023. This present report showcases the development of the method and presents a general workflow for utilising it.

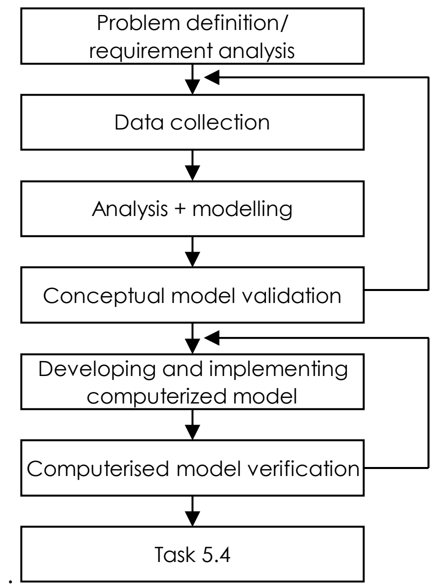

Figure 1: Overview of the methodological approach

2 PROBLEM DEFINITION AND REQUIREMENT ANALYSIS

First, KLU performed a requirement analysis to understand the needs and expectations of potential users of the Reverse Cycle Reverse Logistics Design and Evaluation Method. The analysis consisted of workshops and interviews with partners from the recycling companies within our consortium. Before each discussion, KLU described the general idea of the tool. They then asked the industry and consulting partners to describe (a) how they are currently conducting supply chain planning in their company and (b) how the tool should be designed to support them in the planning. Table 1 shows the requirements revealed by the discussions.

The results of the requirement analysis show that the potential users of the method have a wide range of requirements. These were grouped into (i) input, (ii) output and (iii) characteristics of the tool.

(I) Under input, KLU grouped all scenarios that the recyclers would like to analyse using these tools. This group contains the elements of the model that users wished to manipulate. One element identified was the supply chain design – the recyclers would like to understand how, for example, the change of suppliers or the inclusion of a new customer affects the supply chain. Additionally, the recyclers would like to alter the material flow to determine, for example, whether the current supply chain setup can deal with changes in the material composition. They were also interested in how the use of different trucks would impact the supply chain. One constraint the recyclers asked to include are transboundary shipment permits. These permits are required to ship waste (e.g., mixed plastics) across the border. It takes three to six months to acquire such a permit and they are only valid for one specific waste product, from one specific origin (company and address) to one specific destination (company and address). Any change in the supply chain automatically requires a new permit. The recyclers mentioned specific characteristics for the different supply chain entities that are especially relevant for them, including operational costs and the efficiency of the sorting process. Finally, the recyclers mentioned two dynamics for inclusion in the model: seasonality of supply and demand; and shocks – for example, a sharp increase or decrease in waste supply.

(II) Under output, the performance indicators that the recyclers would like to use to evaluate the differences between scenarios were grouped. These include the revenue of an entity and the cost of transportation. Revenue is a common performance indicator. The cost of transportation is especially relevant in recycling, as it represents approximately one-third of the recycling costs. Additionally, recyclers would like to use the tool to maximise the output of the recycling process and revenue. They would also like to use the tool to identify possible improvements in their current operations.

(III) Concerning the characteristics of the tool, the recyclers mentioned that they would like it to be low cost and easy for their employees to use.

This requirement analysis was an essential step in the development of the tool. KLU used the identified requirements as the basis for the decisions during the tool's development – for example, regarding the selection of the most suitable software and the necessary functionalities.

Table 1: Recyclers' requirements regarding the method

Input	• Altering supply chain design
	  ○ Open/close facilities
	  ○ Add/remove customers
	  ○ Add/remove suppliers
	  ○ Relocate facilities
	  ○ Set opening and closing cost of facilities
	
	• Altering material flow
	  ○ Include difference in quality, e.g., from different suppliers
	  ○ Add new/change sorting process
	  ○ Include changes in waste stream composition
	  ○ Create a specific quality for a specific customer
	  ○ Alter ordering strategy
	  ○ Alter storage and delivery strategies
	  ○ Include different modes of transport (i.e., trucks)
	  ○ Take into account transportation constraints (e.g. transboundary shipments)
	
	• Altering characteristics of supply chain entities
	  ○ Alter cost of operations
	  ○ Alter throughput at facility
	  ○ Change efficiency of sorting processes
	
	• Better understanding influence of dynamics in market
	  ○ Ability to simulate seasonality
	  ○ Ability to simulate shocks

Output	• Calculate cost of transportation • Calculate revenue • Maximise output • Maximise revenue • Identify room for improvement
Characteristics of the tool	• Low cost • Easy to use

3 CONCEPTUAL MODEL DEVELOPMENT AND VALIDATION

The conceptual model is designed to capture different types of supply chain setups. KLU based its development on the results reported in the CREAToR deliverable “D5.1. Mapping of best practices for reverse cycle logistics”[11] Additionally, data was collected from CREAToR’s industrial partners and from the literature to understand possible variations in recycling supply chains. Two workshops were conducted to validate the conceptual model.

3.1 DEVELOPMENT OF CONCEPTUAL MODEL

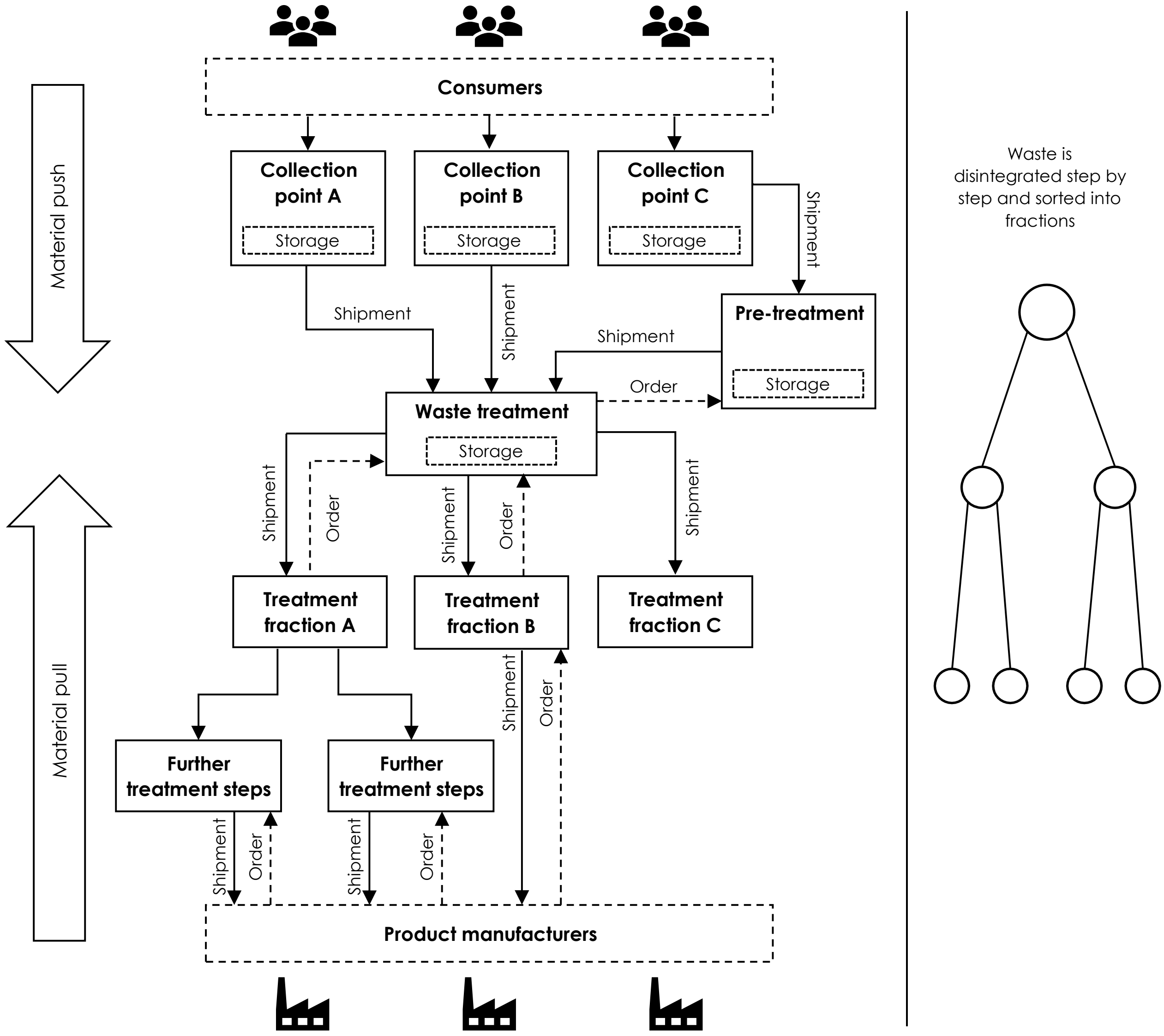

Figure 2: Conceptual model of recycling supply chain

The conceptual model captures elements typical of a post-consumer recycling supply chain. The setup only changes slightly for a post-industrial or B2B recycling supply chain. In this case, the initial input

[11] Moritz Jäger-Roschko et al., ‘Challenges and Best Practices in Recycling Supply Chains: A Qualitative Analysis of Five Major Waste Streams’, *SSRN Electronic Journal*, 2020, https://doi.org/10.2139/ssrn.3715565.

comes from other companies rather than the consumer. While every supply chain is different in design, the conceptual model captures elements typical for recycling supply chains and distinguishes a recycling supply chain from a forward or manufacturing supply chain. These elements are essential for the development of the model as they do not exist in forward supply chain simulation models. KLU did not aim to capture every potential variation of recycling supply chains. Instead, they sought to understand the most important elements and dynamics to ensure that these were represented via the chosen modelling technique and software. Additionally, the research for the conceptual model underlined the complexity and specificity of recycling supply chains, even those treating the same EOL product. It was therefore decided to use a flexible model and thus enable the recyclers to build a digital twin including all the particularities of their supply chain, allowing an easy application of the results.

The split into material push and material pull tiers is a particular feature of recycling supply chains. The consumers typically dictate the first steps, as the amount and quality of the discarded products determines the input for the recyclers and leads to fluctuations in supply quantity and quality. This material push from consumers is present in the first tiers of a recycling supply chain. At some point, the dynamics shift, and the firms' operations are then determined by the demand of product manufacturers, passed from firm to firm along the supply chain. The disintegration that occurs from step to step is another peculiarity that sets the recycling supply chain apart from a manufacturing supply chain. In a manufacturing supply chain, the products begin as parts and are assembled along the supply chain. In a recycling supply chain, whole products or packaging containing multiple materials are collected from the consumer. At every step in the supply chain, the waste is disintegrated further, leading to purer but smaller fractions. Finally, even in the first tiers, fractions are sometimes pulled from other firms – for example, to fill the plant's capacity. Some fractions may be pushed down the supply chain by a firm, while others are pulled by downstream customers. These are mostly side streams and waste fractions. Side streams are fractions that make up only a few percent of the recovered material and are, therefore, not the main business of the recycler. Waste fractions are fractions for which there is no demand further down the supply chain, and which are therefore sent for incineration.

3.2 VALIDATION OF CONCEPTUAL MODEL

While developing the conceptual model, KLU sought to understand the dynamics of recycling supply chains to ensure data validity. For this purpose, an extensive study of various recycling industries was carried out using interviews and other data sources (see D5.1). Additionally, the WEEE recyclers within the consortium, Coolrec (CLR) and Treee (REL), actively contributed to the development of the method, providing regular feedback during the different steps of the model development and input to model the recycling supply chain processes. To validate and verify the simulation model, Sargent's[12] three steps of conceptual model validation, computerised model verification and operational validation (see Figure 3) were followed. In this report, KLU validates the conceptual model and verifies the computerised model (see Figure 3, complete circle). In task 5.4, KLU will validate the data and ensure operational validity via a use case relevant for the CREAToR project (see Figure 3, dashed circle). The conceptual model validation will be described in the following section. The computerised model verification is described in section 4.3.

[12] 'Verification and Validation of Simulation Models', *Journal of Simulation* 7, no. 1 (2013): 12–24, https://doi.org/10.1057/jos.2012.20.

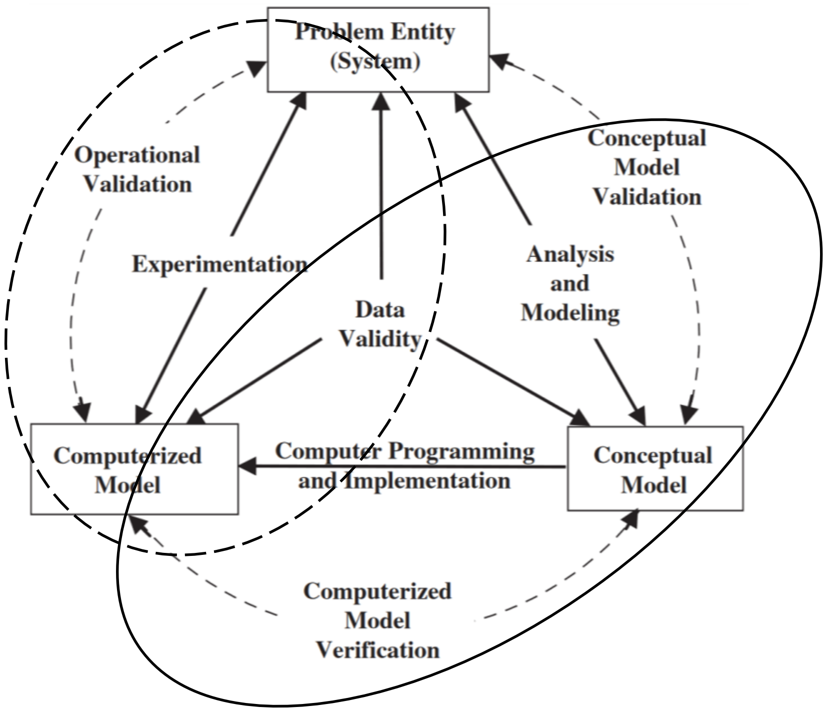

Figure 3: Validation and verification concept for Reverse Cycle Design and Evaluation Method (Source: Sargent[13])

“Conceptual model validity determines that (1) the theories and assumptions underlying the conceptual model are correct and (2) the model’s representation of the problem entity and the model’s structure, logic, and mathematical and causal relationships are ‘reasonable’ for the intended purpose of the model.” [14]

To achieve conceptual model validation, KLU conducted two workshops with experts from the recycling industry. During these workshops, the researchers from KLU presented the conceptual model in detail using flowcharts and other visualisation tools. Additionally, they used structured walkthroughs to explain the model step by step to the experts. The goal of the workshops was to obtain face validity. The experts joining the workshop had to judge whether the model and its behaviour were a reasonable simplification of reality. For example, was the logic of the conceptual model correct, and did it include all the key processes? These presentations led to detailed discussions with the recycling experts to pinpoint inaccuracies in the model. During the first workshop in mid-September 2021, the model lacked some aspects. KLU therefore updated the model and organised a second validation workshop in early October 2021. During the implementation of the model in the computer program, an event validity test and traces were also carried out to verify that the desired mechanisms were correctly implemented in the model.

[13] Sargent.

[14] Sargent, 17.

4 COMPUTERISED MODEL DEVELOPMENT AND VERIFICATION

Based on the requirements highlighted by the recyclers and the conceptual model developed, KLU created a simulation tool that allows a 'what if?' or scenario analysis of supply chains. They chose a simulation tool because it allows the inclusion of stochastic elements, seasonality and the interaction of different supply chain entities, which cannot be included in optimisation tools such as linear programming [15]. Additionally, the simulation allowed the effect of different storage and shipment policies to be investigated in detail, especially concerning logistics. The practitioners identified these aspects as particularly important.

4.1 SOFTWARE SELECTION

KLU selected the software based on two main criteria: flexibility and ease of use. For the recyclers, it is crucial to model individual recycling supply chains to understand how potential changes such as the inclusion of a new supplier will affect operations. The setup of every recycling supply chain is different. The tool therefore needed to be flexible and not too stylistic so that the details of the recycling supply chain could be included. Additionally, the tool will be used by recycling company employees, many of whom are not modelling experts. The tool should therefore be easy to use, and its use should be well documented.

Existing models and tools that could be used as a basis for the method were investigated. The existing models in the academic literature tend to be stylised and poorly documented. These models often include a limited set of actors and focus on a particular supply chain setup. Considerable experience in the specific method is necessary to adapt these models. KLU therefore also explored existing tools for the simulation of supply chains. Two tools for in-depth analysis were selected: the *Supply Chain Guru* from Coupa (formerly Llamasoft) and *anyLogistix* from the AnyLogic company. These two tools are the most popular, and most closely fit the CREAToR requirements. KLU implemented a simple three-tier recycling supply chain prototype using both environments to test their functionality. It was decided to use a*nyLogistix* as the basis for the computerisation of the model, as its intuitive interface makes it easy to use. The range of functionality is mostly the same. Both allow the modelling and simulation of very detailed supply chain digital twin with a lot of possibilities for customization.

AnyLogistix can be used to design, optimise and analyse supply chains. The software contains tools to analytically solve greenfield analysis (location allocation) problems and enable supply chain master planning using linear programming. Additionally, it contains a simulation engine based on AnyLogic's discrete-event simulation engine. The software tool is flexible and allows the user to build a digital twin of the real-life supply chain and then implement changes to the digital twin to test different scenarios. It already addresses crucial elements of supply chain planning, including customer, warehouse, factory, supplier and the mechanisms and tools to connect and modify these entities to align to the user's needs. However, the tool is designed to simulate manufacturing and retail supply chains with a material flow from raw material via production to the consumer. The following section describes how the tool to simulate a recycling supply chain, as described above, was adapted.

4.2 COMPUTERISED MODEL

The computerised model allowed the creation of a digital twin of a recycling supply chain. To explain the essential elements of the computerised model, a simple prototype of the first three tiers of an e-waste recycling supply chain was developed. This setup would be chosen by a primary treatment facility to analyse its supply chain. The test model contained three municipal collection facilities that ship their material to the primary treatment facility, where the material is shredded and sorted into three fractions: metal, plastics and waste. The first two items are then shipped to the corresponding treatment facilities, and the waste is incinerated (see Figure 4)

[15] Iris Heckmann and Heckmann, *Towards Supply Chain Risk Analytics* (Springer, 2016).

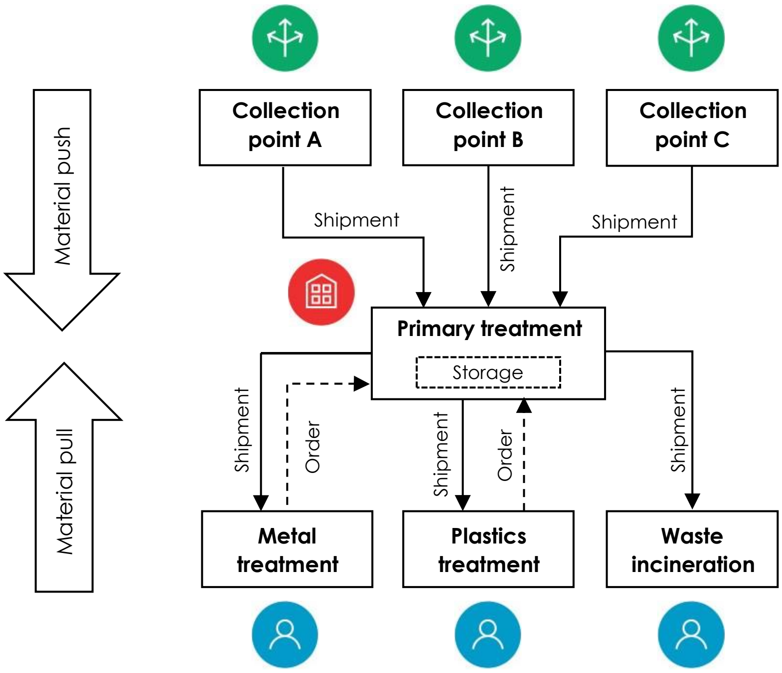

Figure 4: Three-tier e-waste recycling supply chain used to test the model

Model implementation

One visual output of *anyLogistix* is the GIS (geographic information system) map. This map can be used to create, move and delete supply chain entities. It also shows the connection of the different elements in the model. To simulate transportation between the supply chain entities, *anyLogistix* uses data provided by OpenStreetMap to calculate distances.

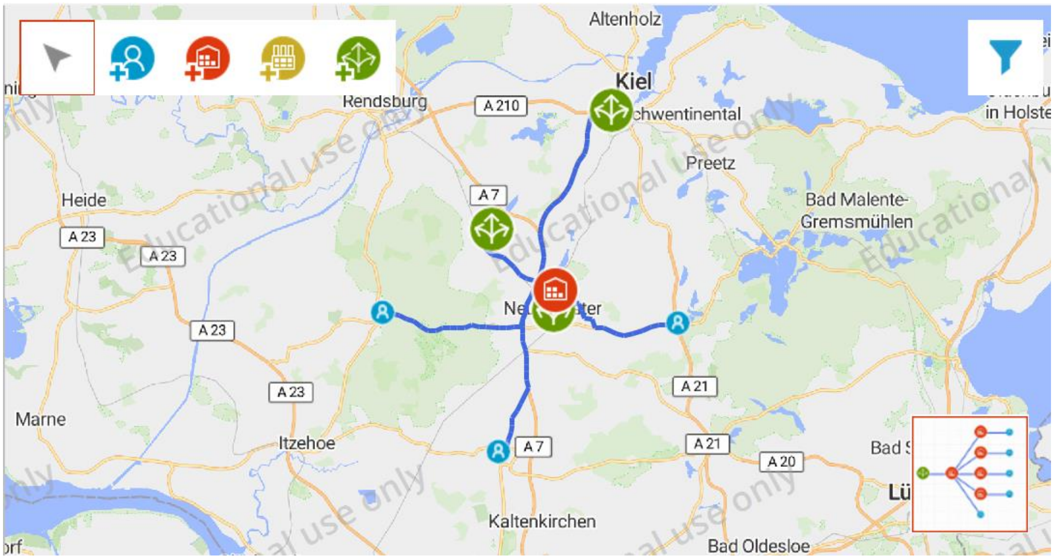

Figure 5: GIS map displaying a three-tier recycling supply chain (screenshot from anyLogistix)

The core of the anyLogistix software is the tables used for data input and configuration of the model. This section explains which tables were used to implement our simple test model and what options for recycling supply chains they provide. These tables cover all essential properties necessary to set up the digital twin of a recycling supply chain. At the end of this section, we introduce possibilities for extending the model by making it more detailed and adding more data for additional analysis.

The first tables to complete when creating a supply chain model are those for suppliers, factories and customers. For a recycling supply chain, the entities behind the elements differ slightly from the category labels. A supplier is the first tier in the model, and for our purposes this is the collection points. The factories are recycling facilities, which in our case means the primary treatment facility for shredding and sorting the EOL products into metal, plastics and waste. The customers are the last tier of the supply chain. In CREAToR's case, these are the metal and plastics treatment facilities and the waste incineration. The model allows warehouses or distribution centres to be added, but this is not necessary in our case, as the factories already contain a warehouse where incoming and outgoing materials are stored.

In the tables, the location of the entities can be set as shown on the GIS map. In addition, for the factories, a maximum capacity can be defined.

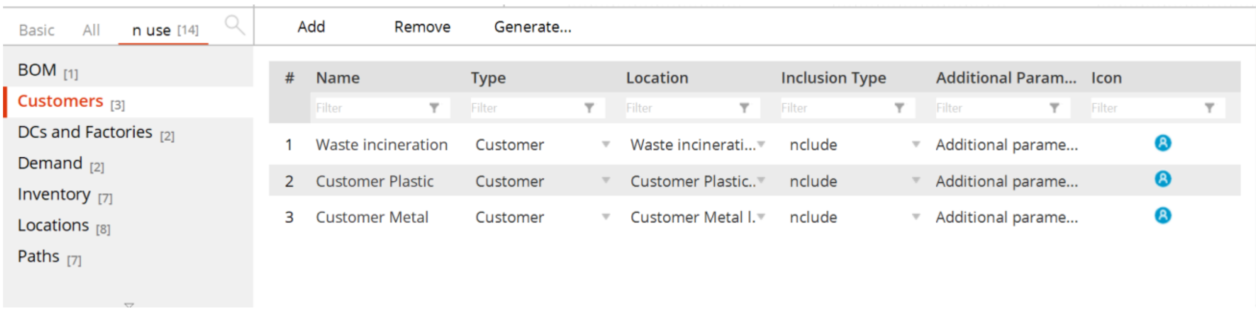

Figure 6: anyLogistix tables used for data input (screenshot from anyLogistix)

The path table is used to connect two elements in the supply chain, allowing a product to be transported from one location to another. This table also allows the rules for calculating transportation costs to be defined. Among other options, the cost can be fixed based on the number of products delivered or the distance of the path. If multiple types of vehicles operate on this route – for example, walking floor and normal trailers – a path has to be set up for each vehicle type. If desired, the user can also set rules for CO_2 calculation in this table. Underlying the path table is the vehicle table where the user can define different types of vehicles, including their capacity (either in volume or weight) and average speed.

The inventory table is used to define the inventory policy for the recycling facilities. The user can choose between multiple common inventory policy types such as min-max policy with and without safety stock, RQ policy, regular policy or order-on-demand. For each policy, the relevant parameters can be defined, including reorder point, order quantity or reorder interval.

The production table is used to define what sites produce which product or, in the case of a recycling supply chain, the steps of the recycling process. The production process is defined in the BOM (bill of materials) table. The BOM table is designed as a list of components needed to assemble an end product. The table, however, also contains a list of by-products. If a sorting process is being modelled, it must be put into the system as follows. The incoming products or fractions are put into the software as components. One outgoing fraction is put in as the end product, the others as by-products. In our case, the e-waste is the input from the collection points, so we set them as components. After shredding and sorting, the three categories of metal, plastics and waste are obtained. Hence, waste for incineration was implemented as the end product, with metal and plastics as by-products. The share of each material that can be recovered is also defined in this table. Multiple qualities of waste composition can be defined via this table – for example, for different collection groups of e-waste or different suppliers. It can also be specified whether the waste composition changes over time. Additionally, the processing time can be defined in the production table specifying the production time per unit or, in our case, the tonnes of material treated per hour.

The demand table defines the demand from each customer. The demand can be defined as a periodic demand or as an external input. The periodic demand is demand of a repetitive nature that reoccurs in the same quantity at a regular interval – for example, 10 tonnes every month. The program also allows stochastics to be added to the periodic demand as it can occur on a random day in the selected interval, or the quantity is defined via a probability distribution. Alternatively, the demand can be introduced via an external table. This external table can contain historic demand collected by the company over recent years. It can also contain forecasted demand that accounts for more complex logics not available in the program itself, such as seasonality. AnyLogistix assumes that the demand is generated by the last tier in the model - in our case, the metal and plastic treatment facilities - and then trickles down the supply chain. For the analysis of a recycling supply chain, it can be helpful to analyse the interaction of the material push and the material pull in the different sections of the supply chain and determine whether, despite stochastic effects and other fluctuations in supply and demand, the warehouses and stock levels are sufficient.

In the shipping table, the user defines the shipping policies for the various materials and routes (from one entity to another). The main policies that can be selected are LTL (less than truck load), FTL (full truck load) and push. With FTL policy, the orders will only be shipped if the truck is filled to the minimum load ratio. With LTL orders, any amount can be shipped. With the push policy, demand is taken to the required destination regardless of demand. The push shipment can be triggered if a site's inventory reaches its limit. Additionally, the shipments can also be defined by a schedule. In the CREAToR case, LTL/FTL for the shipment from the primary treatment facility to the metal and plastics treatment facility is used as the treatment facilities have a demand that needs to be fulfilled and are therefore pull shipments. A scheduled push policy for shipment from collection points to primary treatment is used for this case. As the material is pushed into the supply chain by the consumers, there is no demand from the primary treatment facility to consider. The schedule can be created outside of anyLogistix, based on historic supply data or other forecasts to match expected supply considering, for example, seasonality or other events such as an increased supply of e-waste due to sales by big retail brands. KLU used the uniform push policy for shipping between primary treatment and waste incineration. Every time a full truckload of waste is in the recycler's warehouse, it will be shipped to the incineration facility.

The sourcing table defines sourcing policies. In the event of multiple supply chain entities delivering the same product, the user can define the source. Possible sourcing policies are cheapest (regarding transportation costs), closest, fastest and split sourcing. In the case of e-waste these can be relevant for the sourcing of B2B input and to model the dynamics in a multi-tier supply chain.

Additional tables allow further analysis of the supply chain. The extensions readily available in anyLogistix are CO_2 calculation for transport and facilities (via CO_2 from facilities/processing), shocks (via events), processing cost and time – for example, for unloading, (via processing cost and processing time).

Running the experiments

AnyLogistix allows different experiments to be performed. In a standard simulation experiment, the implemented scenario can be executed for the chosen amount of model time, using the AnyLogic discrete-event engine to simulate the behaviour of each supply chain entity based on the design and policies defined by the user. While the simulation is running, the user can observe the deliveries on the GIS map and check the exact number of orders placed, products produced and stock levels of any facility to understand the system's dynamics. Additionally, data is gathered for real-time analysis. This data is also stored and can be analysed in anyLogistix or exported to other programs for a more detailed visualisation and analysis. Many performance indicators can be used to analyse the scenarios (e.g., revenue, transport cost, production cost, inventory levels, orders placed, products produced). For these performance indicators to be meaningful, the experiments must be set up to ensure that the main contributing factors are included in the model – for example, cost and revenue.

Additional, more advanced, experiments can be run in anyLogistix, including variation, safety stock and risk analysis experiments. The variation experiment comprises a series of simple experiments. Over the series, one or more parameters are varied. These experiments can be used to understand how changes in one parameter affect the supply chain. The results comprise one run for each parameter setting, allowing a comparison of the different settings. The variation experiment can also be used if the model comprises stochastic elements. Multiple simulation runs can then be completed to produce statistical significance. Safety stock experiments help the user determine the safety stock necessary to maintain the desired service level throughout the supply chain despite stochastic influences. In a risk analysis experiment, the user can implement random or expected shocks or events such as the breakdown of a facility or sudden changes in supply or demand to test the resilience of the supply chain.

4.3 VERIFICATION OF THE COMPUTERISED MODEL

> *"Computerized model verification ensures that the computer programming and implementation of the conceptual model are correct."* [16]

KLU performed a computerised model verification to ensure that the computer programming and the implementation of the conceptual model were correct [17]. The computer programming itself was not problematic in this case since KLU used a special-purpose simulation environment. However, KLU still had to ensure that they employed the environment correctly and that the external data they fed into the model was compatible with the program. Additionally, they had to verify that the mechanisms of the conceptual model were correctly implemented in the computerised model. The techniques used to verify the computerised model were: traces, following the behaviour of specific elements through the model (e.g., from orders to production to shipment); investigation of the input-output relationship, to understand how changing certain input variables such as shipping policy or order quantity affected the model; and data relationship correctness, to check whether the values the system calculated and collected during the simulation were correct. Additionally, KLU used extreme condition tests, using very low (0) and very high numbers to see if the system reacted correctly; and an internal validity test, producing several replication runs to determine the amount of stochastic variability.

[16] Sargent, 'Verification and Validation of Simulation Models', 18.

[17] Sargent, 'Verification and Validation of Simulation Models'.

5 WORKFLOW REVERSE CYCLE DESIGN AND EVALUATION METHOD

KLU developed a six-step workflow based on Law's[18] flowchart for a simulation study. KLU's method involves six steps to build a digital twin and run a scenario analysis (see Figure 7). The necessary steps are described in this section.

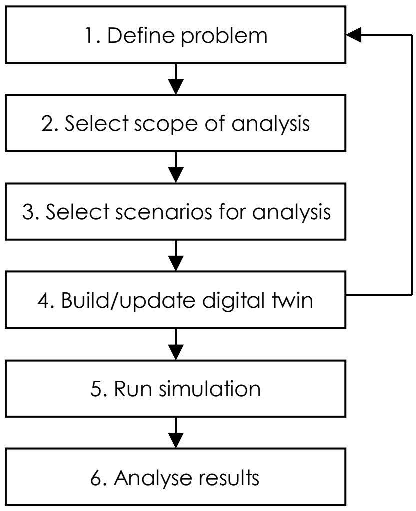

Figure 7: Workflow of Reverse Cycle Design and Evaluation Method

1. Define problem

First, the managers of the recycling company need to formulate a problem of interest. This problem must be formulated precisely and related to issues of supply chain design to be suitable for analysis using the proposed method. The process is usually not linear, which means that problems with the initial problem definition will arise during the later steps of the analysis. The problem definition then needs to be altered to make it more precise or a better fit for the tool. Ideally, the prepared problem statement contains (i) the overall objective of the study and (ii) specific questions to be answered through the analysis.

(I) The overall objective of the study sets the general expectations of the analysis and can be used to derive more specific elements such as questions, scope and scenarios.

(II) The specific questions are crucial, as they guide the subsequent steps. They must therefore be chosen carefully. One effective method is to formulate the questions in the form of 'how does X affect Y?', where X is one of the input variables and Y is one of the output variables or performance indicators evaluating the efficiency of each scenario. The following questions are provided as an example:

- Do I have enough capacity to add another supplier?
- What fleet size do I need to reach service level X?
- How would it affect my revenue if I switched to a different supplier?

2. Select scope of analysis

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[18] Averill M. Law, *Simulation Modeling and Analysis*, Fifth edition, McGraw-Hill Series in Industrial Engineering and Management Science (Dubuque: McGraw-Hill Education, 2013), 66–70.

The problem statement defines the scope of the analysis and determines the supply chain tiers included in the model. It is possible to include only two tiers in the model – for example, suppliers and the focal company. However, it is often practical to include at least three tiers in the model (e.g., suppliers, the focal company and the customer) to fully understand the supply chain dynamics. For a recycler conducting a supply chain analysis, it can be difficult to include more tiers, as the necessary data for suppliers and customers – for example, concerning their operations – are often unknown. Models with a more extensive scope need more input data, which leads to a less detailed analysis. This is not a disadvantage per se; however, the scope and level of detail chosen must be aligned to the problem statement if the questions guiding the analysis are to be answered.

3. Select scenarios for analysis

The user needs to decide on the scenarios for analysis. For each question defined in the problem statement, at least one scenario must be defined. Each scenario is an alteration of the digital twin representing the status quo supply chain. It is necessary to run a scenario for each change in the status quo to understand the influence of those changes. If multiple changes are made to the model – for example, by changing the types of trucks used and the location of a supplier – it might not be clear why the transportation costs are increasing. The tool also offers a variation experiment to analyse the influence of a particular parameter such as fleet size or facility capacity by altering this parameter and then investigating the impact on the performance indicators of interest. The selection of scenarios is also crucial, as it defines in combination with the problem statement the minimum level of detail the digital twin requires.

4. Build or update digital twin

The development and implementation of the digital twin require the collection of significant quantities of data. Depending on the scope and scenarios selected, this data might come from the company using the method or from other firms along the recycling supply chain. However, in most cases, the data available in the companies' system will not directly match the required input for the model. In this scenario, the data needs to be converted (e.g., aggregated). If no matching data are available, experts from the company can take an educated guess. If assumptions are used, it is practical to run a sensitivity analysis with these parameters based on the assumptions. By increasing and decreasing the assumed values, the modeller can gauge the impact of possibly wrong assumptions. If the desired values cannot be collected, it might be necessary to alternate the analysis and redefine the problem. In every case, it is practical to build a simple model first, test whether it works, and then slowly increase the complexity of the model step by step.

5. Run simulation

After developing the digital twin, the user needs to run the simulation. First, the status quo version is run to establish a baseline and validate the model. If the model behaves as expected and the numerical results are satisfactory, the scenarios can be run. For every scenario selected, the model needs to be adapted – for example, by editing the supply chain design or the parameters of the different entities. If the user wants to test specific parameters, they can run a variation experiment that alters the parameter in question.

6. Analyse results

An initial analysis of the results can be performed using the anyLogistix dashboard. For a more complex analysis and visualisation of the results, the data should be exported. Data analysis tools such as R, Python or SPSS can then be used to run more sophisticated algorithms – for example, an ANOVA (analysis of variance) – to understand the significance of the changes made across the different scenarios. Based on the analysis results, the managers of the recycling supply chain can evaluate the various scenarios and make informed decisions to improve their supply chain and operations.

6 CONCLUSION

The Reverse Cycle Design and Evaluation Method is a flexible tool that allows managers along the recycling supply chain to perform a 'what if?' analysis with a digital twin of their supply chain. The method incorporates most aspects judged important by practitioners.

Regarding input, the tool is flexible and allows the design of the supply chain to be altered easily – for example, via the GIS map. It is therefore no problem to add or remove suppliers and customers and relocate facilities. Altering the material flow is not possible on a process level since the tool does not model the material flow in the facilities but rather considers the entire supply chain. The facilities themselves are black boxes. Instead, the changes are implemented one level above. To include a new sorting process, a new BOM must be added to implement the changes in yield of the improved sorting line. Additionally, the processing costs and throughput must be altered accordingly. Specific requests from customers about quality cannot be considered automatically. Instead, the processing needs to be manually adjusted – again using BOMs to produce the requested quality. Different waste compositions or qualities, however, can be considered. It is possible to alter ordering, and storage and delivery strategies for each actor in the supply chain individually. The user can also constrain the transportation by setting up specific paths defining from which and to which entity transportation is allowed. This, for example, allows the user to specify which transboundary routes can be taken for which waste stream using which type of vehicle to model the constraints of the transboundary shipment permits. The characteristics of the supply chain entities such as cost, throughput or yield can easily be modified. Moreover, seasonality, shocks and stochastic elements can be included to better understand the dynamics of the recycling supply chain.

Concerning output, the tool allows a broad range of different performance indicators to be collected to determine the characteristics of each scenario, including transportation cost and revenue. However, the tool is based on simulation. Hence, it allows the comparison of different scenarios to ascertain which one will generate the highest revenue or output. Direct optimisation is not possible. The ability to analyse the behaviour of the supply and multiple parameters while the simulation is running allows the user to better understand the dynamics of the supply chain and identify room for improvement.

The tool is user-friendly, as it has a very intuitive interface and is well documented. As KLU's solution is based on existing software, it will also be maintained in the future. If the tool is cheap is hard to judge, and each company should conduct its own cost-benefit analysis.

Table 2: Comparing the method's capabilities and the recyclers' requirements

	Recycler's requirements	Degree of integration
Input	• Altering supply chain design	●
	○ Open/close facilities	●
	○ Add/remove customers	●
	○ Add/remove suppliers	●
	○ Relocate facilities	●
	○ Set opening and closing cost of facilities	●
	• Altering the material flow	◕
	○ Include difference in quality, e.g., from different suppliers	●
	○ Add new/change sorting process	◑
	○ Include changes in waste stream composition	●
	○ Create a specific quality for a specific customer	◑
	○ Alter ordering strategy	●
	○ Alter storage and delivery strategies	●
	○ Include different modes of transports (i.e., trucks)	●

	○ Take into account transportation constraints (e.g. transboundary shipments)	●
	• Altering characteristics of supply chain entities	●
	○ Alter cost of operations	●
	○ Alter throughput at facility	●
	○ Change efficiency of sorting processes	●
	• Better understanding influence of dynamics in market	●
	○ Ability to simulate seasonality	●
	○ Ability to simulate shocks	●
Output	• Calculate cost of transportation	●
	• Calculate revenue	●
	• Maximise output	◑
	• Maximise revenue	◑
	• Identify room for improvement	◕
Characteristics of the tool	• Low cost	◑
	• Easy to use	●

The method KLU has developed will be a helpful tool for managers in the recycling supply chain. It allows users to test alternative supply chain designs and supply chain innovation, understand the dynamics and interdependencies of their supply chain and perform a risk assessment. Recycling supply chains contain many uncertainties. Using the stochastic elements included in the dynamic simulation helps assess the risk of running out of stock and assess suitable fleets or warehouse size. Most importantly, the simulation environment allows recycling managers to conduct 'what if?' analyses in a risk-free environment. As the recycling industry is rapidly growing, many changes have to be made regarding supply chains and investment decisions. Dynamic simulation can help managers understand their operations and supply chain and thus make informed decisions.

This document can be used as a user guide to employ the Reverse Cycle Design and Evaluation Method. The general process is described step-by-step in the workflow in chapter 5. More specific instructions for the implementation of the model in the software can be found in section 4.2. Here the specific steps to develop a digital twin of a recycling supply chain using anyLogistix are explained. The technical performance indicators as defined by the project have been successfully met. A conceptual model of the recycling supply chain (see section 3.1) has been proposed. The method has been developed and implemented using anyLogistix (see section 4.2). Finally, the conceptual model has been validated using expert workshops (see section 3.2) and the computerised model has been verified using, for example, extreme condition tests (see section 4.3).

As a next step, KLU will use the Reverse Cycle Design and Evaluation Method to conduct a case study with the CREAToR industrial partner Treee. Performing this analysis will help to validate the method further and should yield insightful results for the partner and the project. The model will be used to analyse where additional facilities are needed, what size they should be and how the material flow between the facilities should be implemented when the CREAToR technology is introduced onto the market. The results from the model are expected to provide a detailed breakdown of the cost and revenue streams resulting from operating CREAToR sorting and purification technology. The volume of polymer waste needed, and its sourcing, are of particular interest. As logistics costs represent a high share of overall recycling costs, it is crucial to understand their variability and sensitivity based, for example, on the size of the CREAToR facility. These results will be reported later in the project (March 2022) in the deliverable D5.4 "Specific reverse logistics concept for CREAToR materials".

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