



A systems engineering framework for the optimization of food supply chains under circular economy considerations

Stefanos G. Baratsas^{a,b}, Efstratios N. Pistikopoulos^{a,b}, Styliani Avraamidou^{b,*}

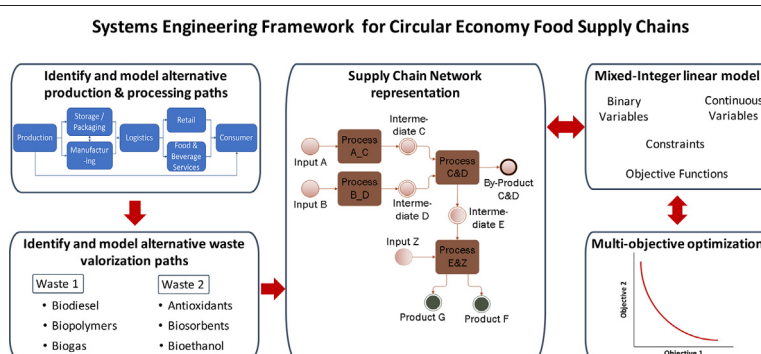
^a Artie McFerrin Department of Chemical Engineering, Texas A&M University, Jack E. Brown Chemical Engineering Building, 3122 TAMU, 100 Spence St., College Station, TX 77843, United States

^b Texas A&M Energy Institute, Texas A&M University, 1617 Research Pkwy, College Station, TX 77843, United States

HIGHLIGHTS

- A novel framework to model and optimize circular economy food supply chains
- Superstructure representation and optimization to obtain circular supply chains
- Trade-off analysis of circular economy conflicting objectives

GRAPHICAL ABSTRACT



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ABSTRACT

The current linear “take-make-waste-extractive” model leads to the depletion of natural resources and environmental degradation. Circular Economy (CE) aims to address these impacts by building supply chains that are restorative, regenerative, and environmentally benign. This can be achieved through the re-utilization of products and materials, the extensive usage of renewable energy sources, and ultimately by closing any open material loops. Such a transition towards environmental, economic and social advancements requires analytical tools for quantitative evaluation of the alternative pathways. Here, we present a novel CE system engineering framework and decision-making tool for the modeling and optimization of food supply chains. First, the alternative pathways for the production of the desired product and the valorization of wastes and by-products are identified. Then, a Resource-Task-Network representation that captures all these pathways is utilized, based on which a mixed-integer linear programming model is developed. This approach allows the holistic modeling and optimization of the entire food supply chain, taking into account any of its special characteristics, potential constraints as well as different objectives. Considering that typically CE introduces multiple, often conflicting objectives, we deploy here a multi-objective optimization strategy for trade-off analysis. A representative case study for the supply chain of coffee is discussed, illustrating the steps and the applicability of the framework. Single and multi-objective optimization formulations under five different coffee-product demand scenarios are presented. The production of instant coffee as the only final product is shown to be the least energy and environmental efficient scenario. On the contrary, the production solely of whole beans sets a hypothetical upper bound on the optimal energy and environmental utilization. In both problems presented, the amount of energy generated is significant due to the utilization of waste generated for the production of excess energy.

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* Corresponding author.

E-mail addresses: sbaratsas@tamu.edu (S.G. Baratsas), stratos@tamu.edu (E.N. Pistikopoulos), styliana@tamu.edu (S. Avraamidou).

1. Introduction

Rising populations across the world (UN, D, 2019) seek to improve their standards of living, placing huge stresses on natural resources and supply chains (Mukhi et al., 2020). Energy and operational efficiency, improvement in manufacturing processes, quantitative management of food-energy-water nexus (Avraamidou et al., 2018; Deng et al., 2020; Li et al., 2019; Nie et al., 2019), and economic growth are vital to fulfill the increasing demand for goods, food and services (Baratsas et al., n.d.), however they still lead to natural resource degradation (Panayotou, 2016), substantial waste generation (Ferronato & Torretta, 2019), water contamination (Schwarzenbach et al., 2010), and surging greenhouse gas emissions (Alam et al., 2016; Chen et al., 2016; Lee et al., 2017; Tiba & Omri, 2017). Thus, economic expansion shall be combined with sustainable development, ensuring the advancement of our societies while preserving the environment (Bergstrom & Randall, 2016; Sarkodie et al., 2019; Zaman & Abd-el Moemen, 2017). This requires a fundamental transformation of our economic model (Westley et al., 2011) that promotes the “take-make-use-dispose-pollute” concept to a more “sustainable” one (Andrews, 2015; Stubbs & Cocklin, 2008).

Circular Economy (CE) has emerged as a potential solution for such a transition, with extreme emphasis being put towards improvement in reuse, remake, repair and recycling (Beaulieu, 2015). Korhonen et al. (Korhonen et al., 2018) defines CE as a combination of production-consumption systems that maximizes the output services in a sustainable manner, without violating the natural reproduction rates, while utilizing cyclical material flows, and renewable energy sources and flows. CE aims to solve resource, waste, and emission challenges confronting society by creating a production-to-consumption total supply chain that is restorative, regenerative, and environmentally benign (MacArthur, 2015). Eco-effectiveness, through a holistic optimization of all components, along with a great emphasis on the design and systems thinking, is the main focus of CE (Beaulieu, 2015; MacArthur et al., 2013). The goals and key characteristics of CE (Avraamidou et al., 2020; Reichel et al., 2016) are summarized as follows:

1. Reduction of material losses/residuals: Waste and pollutants minimization through the recovery and recycle of materials and products.
2. Reduction of input and use of natural resources: The reduction of the stresses posed on natural resources through the efficient use of natural resources (e.g. water, land, and raw materials).
3. Increase in the share of renewable resources and energy: Replacement of non-renewable resources with renewable ones, limiting the use of virgin materials.
4. Reduction of emission levels: The reduction in direct and indirect emissions/pollutants.
5. Increase the value durability of products: Extension of product lifetime through the redesign of products and high-quality recycling.

CE can contribute to all dimensions of sustainable development, but it should not be confused with sustainability since they have different goals, motivations, prioritizations, institutionalizations, beneficiaries, time-frames, and sense of responsibilities (Geissdoerfer et al., 2017). The successful and inclusive economic, environmental, and social integration is fundamental for sustainability and sustainable development. Although, the term is quite ambiguous and lacks implementation specificity, it refers and applies to a variety of contexts and time horizons. On the contrary, CE is viewed as an operational tool to enforce sustainability (Kirchherr et al., 2017) through economic prosperity, environmental quality and social equity considering earth as a closed and circular system where economy and environment coexist in equilibrium. Even though the CE concept is still relatively new, with little scientific guidance regarding its successful implementation and its effective evaluation (Corona et al., 2019; Kalmykova et al., 2018), the economic, environmental and social aims are evident from its adoption into national

laws at international and regional levels (macro and meso systems), as well as at the level of private corporations and businesses (micro system). However, the extensive and universal nature of CE introduces significant challenges for the decision-making which are exacerbated from the interconnections among the diverse supply chain elements, stakeholders, and regulatory environments. Therefore, a holistic systems engineering approach is required to quantitatively navigate and thoroughly address the multi-scale, multi-faceted and interconnected CE supply chains (Avraamidou et al., 2020).

1.1. CE food supply chains - (CE FSCs)

Food loss and waste throughout the supply chains represent about one-third of the food that is produced, although more than 820 million people remain chronically undernourished (FAO, 2011). The annual economic costs of this food waste are estimated at \$ 1 trillion, skyrocketing to \$ 2.6 trillion on annual basis when environmental and social costs are accounted for (FAO, F.W.F, 2014). Likewise, the contributions of food loss and waste to climate change are also significant, accounting for about 8% of global greenhouse gas (GHG) emissions (FAO, 2015).

Innovative, collaborative and drastic approaches must be deployed to tackle such a challenging issue. The 2030 Agenda for Sustainable Development from the United Nations has identified and promoted two Sustainable Development Goals (SDGs), particularly SDG 2 and SDG 12 for targeting a Zero Hunger world and ensuring sustainable production and consumption patterns respectively (Assembly, 2015). The implementation of sustainable agriculture will assist towards food security and enhanced nutrition while reducing food loss and waste would result to more efficient land use and improved water resource management with beneficial effects on climate change and livelihoods. Thus, intergovernmental and international collaborations to promote such transformations and advocate new policies are required. Moreover, co-ordination among the various stakeholders of the FSCs with parallel switch of the shopping and consumption habits will accelerate this transition (Esposito et al., 2020).

The concept of CE is of extreme importance in this direction since by definition it is associated with optimization of resources and energy utilization while preserving the environment. CE-FSCs imply minimization of the waste and GHG emissions generated at the various stages of the supply chain. This can be achieved through recovery and recycle, valorization of food waste and by-products as well as by re-using food and recycling nutrients through behavioral change of the consumers, integration of renewables and efficient use of natural resources. Moreover, advanced preservation techniques and reliable storage shall be utilized to increase the lifetime and quality of products. The loop of the nutrients and other materials shall be closed; while the loop of energy shall be open. This “zero-waste” approach is a key differentiating factor between CE and the other sustainability thinking approaches (Veleva et al., 2017).

Governments, industry and academia have demonstrated a growing interest towards CE over the recent years, however it is still at an early stage. Fassio and Tecco (Fassio & Tecco, 2019) conducted a thorough analysis in 40 case studies evaluating the effectiveness of various CE actions towards integration of SDGs into the food systems. Although, the concepts of optimization performance and efficiency along with regenerative and loop actions have emerged, however the practical implementation of CE into the food systems is still missing, while socio-economic and environmental considerations are often omitted. Innovation for circularity and sustainability has become not only a necessity due to climate change and economic environment, but a fundamental for all involved parties to maintain and/or improve their competitive advantage in the 21st century. The intrinsic complexity and comprehensive nature of CE mandates multidisciplinary and collaborative efforts. Process systems engineering (PSE) accompanied by environmental engineering and horticultural sciences could play a crucial role in providing the required tools towards the transition to CE-FSCs (Avraamidou et al., 2020).

To this respect, in this work the foundations of a system engineering framework and quantitative decision-making tool for the analysis and trade-off optimization of interconnected FSCs, governed by the CE principles are presented. The explicit incorporation of CE goals and objectives into the design and operation of FSCs is a key contribution of the proposed framework. FSCs demonstrate unique characteristics, restrictions, objectives and challenges in comparison to the other product or service supply chains. In particular, FSCs consist of several interdependent steps such as farming, processing, distribution, retailing, in a domino type transition. Humans ingest food for nourishment, and as such issues related with perishability, preservation requirements, quality decay, short shelf life and delivery restrictions, necessitate the highest standards of safety and quality for the delivered products (Bortolini et al., 2019). FSCs are also confronted with soaring consumer demand, leading to huge stresses on natural resources and the environment, significant energy requirements as well as substantial waste generation at the various stages. The recent movements towards improved food quality, increased food shipping traceability, along with the emerging ethical dilemmas such as the utilization of biomass for food or fuel and the rising sustainability concerns, set a new scene around the globe, calling for transformational changes across the multi-spatial and multi-temporal FSCs.

The proposed CE-FSC framework combines data and information from the academic and industrial literature, along with mixed-integer modeling to establish the interconnections among different stages of the circular FSCs as well as multi-objective optimization to consider all CE objectives and analyze trade-offs. It is flexible since the set of resources and tasks, as well as the supply and demand information can be constantly updated, reflecting recent trends and developments. Apart from systematically capturing the extensive, up-to-date set of production, processing and valorization pathways, the proposed CE-FSC framework contributes to the literature in a dual manner. First, it enables the identification and selection of the optimal tasks from the list of all alternative processes based on certain CE objectives. On top of that, it allows the identification of the least efficient processes or even sections of the network, which introduce potential bottlenecks within the supply chain. This is a key feature that refocuses the interest and promotes the research and development on the less developed sections of the supply chain. Furthermore, users from a variety of backgrounds can benefit from the proposed framework. Academics and experimentalists could concentrate on the improvement of existing processes or on the creation of completely new ones, while private corporations could evaluate the circularity of parts or their entire supply chains. Governmental policymakers could determine areas that require improvement, and thus promote legislative actions and allocate funding towards these areas.

The supply chain of coffee is used as a case study to illustrate the effectiveness and applicability of the proposed framework. The current linear coffee supply chain is transformed into a circular one under different supply and demand scenarios. Due to the competing nature of CE objectives and supply chain's stakeholders, a multi-objective optimization approach is developed, and solved to optimality by generating different pareto fronts. Therefore, the case study highlights the usefulness of the framework as a decision-making tool that incorporates all sets of tasks and resources under various design and operational criteria and conditions.

The rest of the paper is organized as follows: Section 2 introduces the specific problem that is targeted and presents step by step the framework that has been developed. Section 3 describes a detailed application of the proposed framework as a case study for one key food supply chain, the supply chain of coffee. The results of the case study are discussed in Section 4, while the conclusions and future work are summarized in Section 5.

2. Material and methods

The necessity of the transition to a sustainable food system through the application of CE principles has been recognized and discussed in

the literature (Esposito et al., 2020). Potential barriers and promising solutions have been considered, including economic and environmental (Genovese et al., 2017; Slorach et al., 2019), regulatory (Farooque et al., 2019), technological (Ciccullo et al., 2021), and sector specific (van Keulen & Kirchherr, 2021) obstacles. In addition, theoretical and practical insights along with strategic aspects of the CE supply chains in general have also been reviewed (Batista et al., 2018). Business and governmental leaders have initiated collective efforts to accelerate the transition towards CE for the food system and FSCs, by setting objectives, identifying barriers and proposing solution strategies (PACE, 2021). The interest though is focused on the theoretical and qualitative analysis of this transition, primarily for individual supply chains, without providing a holistic, quantitative framework.

The developed framework comes to address this gap through a holistic system engineering approach, enabling the navigation and fully consideration of any multi-scale, multi-faceted and interconnected CE-FSC. It provides a systematic way to identify opportunities for beneficial improvement, and exhaustively explore interactions and trade-offs. Specifically, it addresses the following problem:

“Given a specific food supply chain, the framework determines the optimal production and processing network based on all CE criteria and different supply and demand scenarios.”

The proposed CE systems engineering framework for FSCs consists of five steps. 1) Production and Processing Pathways. This step is used to model all the stages for the production and processing of the existing supply chain, and then identify and assess all the alternative pathways for the production of the desired product. 2) Waste, Loss and By-Products Valorization Pathways. This step involves the identification and assessment of all the alternative pathways for the waste valorization and food losses minimization. 3) Resource-Task-Network (RTN). In this step, a RTN superstructure representation that includes all the various alternative pathways shall be designed. 4) Mixed-Integer Linear Programming (MILP) Model. This step involves the formulation of the MILP model that captures the entire FSC, its objectives and its constraints into a mathematical modeling representation. 5) Single or Multi-Objective MILP Optimization and Assessment. This last step translates the decision-making process into a single or multi-objective MILP optimization problem, allowing for simultaneous consideration of economic, energy efficiency and environmental criteria. The framework is summarized in Fig. 1. Each step is discussed in detail in the following sections.

2.1. Step 1: Production and processing pathways

Agricultural commodities such as crops and livestock are produced when farmers, fishers, and ranchers combine their land, water and labor resources with capital, machinery and manufactured inputs (Council, N.R, 2015). Then, food can be sold either directly to the end-consumers, or is handled and processed by other sectors before being consumed. The optimization of any FSC considering CE goals and objectives, requires the detailed identification and assessment of all possible stages of the supply chain, including any alternative pathways along with the involved resources. The initial step requires the identification of the input, intermediate, and output resources. Then, a superstructure representation of the FSC must be developed that involves all the stages from harvesting and processing to production and distribution of the final desired product(s), including the conversion factors among these stages. Having determined the resources and processes that are required to produce, process and distribute the final product(s), then any alternative pathways that improve circularity have to be identified and incorporated within the supply chain. The exacerbated nutrients and water imbalances among supply chains and countries driven by the increasing demand for nutrients, especially phosphorus, the massive nutrient losses, the water scarcity and pollution, and the globalized

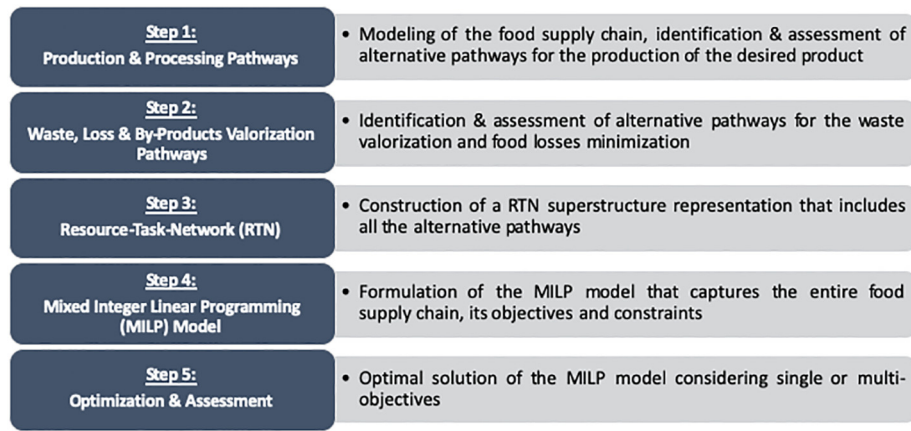


Fig. 1. CE-FSC framework.

structural development of industrialized agriculture (Jurgilevich et al., 2016) must be thoroughly investigated. Under the current linear FSCs, the majority of the waste generated at the different stages are sent to landfills, while the CE-FSC has a zero-waste vision. The goals and key characteristics of CE as described above, should be the guide for this transition towards CE. As such, minimization of the usage of new materials and valorization of wastes through recycling and recovering as well as improving the efficiency of processes or introducing new more efficient ones, should be the priority. New technologies and processes that promote a restorative and regenerative design of FSCs taking advantage of renewable resources and energy must be considered. Having a thorough and inclusive perception of the production and processing pathways of a particular FSC along with the state-of-the-art new developments require a comprehensive literature and business review.

2.2. Step 2: Waste, losses and by-products valorization pathways

In continuation to the previous step, the superstructure representation is extended to capture all the waste, losses and by-products pathways. CE aims to close the material loops and turn the outputs of one supply chain or a manufacturer into inputs for another (Mathews & Tan, 2016), treating waste as a secondary resource (MacArthur et al., 2013). To this direction, it is necessary to have a clear and unambiguous hierarchy of the food waste (FW), surplus (FS) and losses (FL), which will allow the selection of the most environmentally-efficient end-of-life treatment.

The prevention of FS should be the top priority, followed by reuse of food for human consumption and then reuse for animal feed, before considering material recycling, nutrient and energy recovery and having as the last step the food disposal only if it is unavoidable (Teigiserova et al., 2020). However, and despite the efforts, a certain amount of food will end up as waste and/or loss. Thus, it is important to incorporate into the CE-FSC framework the concepts of edibility and possibility of avoidance, which eventually leads to six distinct categories for FS, FW and FL, as proposed by Teigiserova et al.: i) edible - (FS), ii) naturally inedible - (FW), iii) industrial residue - (FW), iv) inedible due to natural causes - (FW), v) inedible due to ineffective management - (FW) and vi) not accounted for - (FL).

Treating waste, losses and by-products as a resource into the CE-FSCs, enables an indefinite use of natural materials and resources (Farooque et al., 2019). An extensive literature and technological review needs to be conducted for the identification and assessment of alternative pathways for the waste and by-products valorization across the supply chain. Technological innovations, superior processes, optimized sequences for the design, processing, packaging, distribution of food products, must be integrated into the original FSCs to ensure the successful implementation of the “zero-waste” goal. By determining the

input - output relationships and the conversion factors among the processes, the energy and material footprints of the FSCs are modeled and calculated. Equally important is the extent of utilization of model approximations within the framework which is directly related to the data availability, data acquisition and handling as well as the degree of acceptance of approximate representations (Demirhan et al., 2021). Various sources could provide significantly different or even contradicting technological, environmental and economic information, thus minimum and maximum limitations are taken into consideration. Ideally, the CE-FSCs would demonstrate alternative pathways that will utilize any waste and by-products for the production of high added value products, such as energy and new materials.

2.3. Step 3: Resource-Task-Network (RTN) formulation

Having completed the identification of the alternative pathways for production, energy and waste valorization, the next step of the CE-FSC framework involves the construction of a Resource-Task-Network (RTN) representation. The RTN representation is a generic and simple mathematical formulation of the interactions between tasks and resources that lead to a bipartite directed graph. Resources include equipment, materials, energy, utilities, manpower, warehouses, distribution locations etc., and are represented as a circle in the RTN, and can be classified as renewable and non-renewable. As non-renewable resources are considered all kinds of materials, utilities, manpower etc., whereas as renewable resources are considered any technological resources in the supply chain network such as production facilities, warehouses, distribution centers, transportation vehicles. Resources are also characterized by their location, enabling the identification of distances between units, which is essential for the modeling of the material transfers within the supply chain network. Therefore, a facility that involves multiple tasks is modeled implicitly, not explicitly, through its associated equipment and technologies at a particular location. A task, represented as a rectangle, is actually an abstract operation that can produce, transform, transport, store, and/or supply resources, with the resources being treated uniformly. As such, tasks may purchase, sell, or store resources, transform one set of resources into another, produce or consume resources at any point of time etc. (Pantelides, 1994). Fig. 2 provides an example of the RTN representation. In this case, Resource1 and Resource3 are consumed in Task 1 for the production of Resource4. Similarly, Task2 consumes Resource1 and Resource4 for the production of Resource6 and so on.

Such a representation enables the modeling of the supply chain resources and tasks as an optimization model, integrating all the design and planning characteristics of the particular supply chain. The resources and tasks along with their interrelationships need to be identified from the postulated set of alternative options. Processing

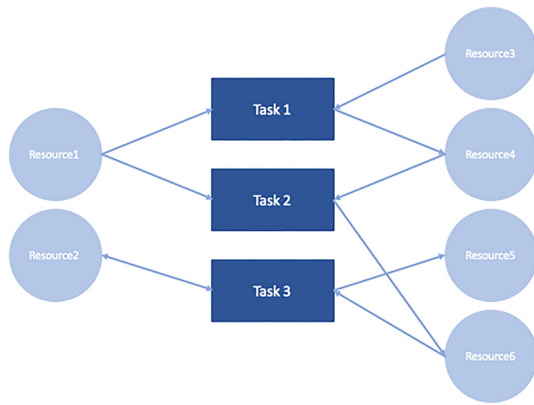


Fig. 2. Resource-Task-Network (RTN) representation (Floudas & Lin, 2005).

equipment units are treated explicitly, which means that units in different conditions e.g. “clean” or “dirty” shall be treated as different resources, although in general, the defining attributes of a resource type depend on the content and the detail of modeling (Kopanos & Puigjaner, 2019; Pantelides, 1994). This superstructure representation provides a generic design methodology that can be applied to any type of FSCs.

2.4. Step 4: Mixed-Integer Linear Programming (MILP) model formulation

Taking advantage of the previous step where the FSC is represented as a RTN superstructure, here this information is translated into a mathematical model of the supply chain. The mathematical model consists of variables, parameters, constraints and mathematical relationships. Variables can take different values reflecting different states of the supply chain. These values can be continuous, integer, or a mixed set of continuous and integers. On the contrary, the parameters have specific, one or multiple, fixed values with each one of those representing different models of the system. Restrictions and limitations of the supply chain are expressed through constraints. The logical conditions among the variables, along with the equality and inequality expressions define the mathematical relationships of the system (Floudas, 1995).

Based on the RTN superstructure representation both continuous and integer variables are required to capture the entire FSC, economic and environmental objectives and constraints. The selection (or not) of any task, meaning any process, technology and/or equipment, within the mathematical model is governed by a binary variable. The same applies for the selection (or not) of a resource, i.e. material, energy etc. Therefore, a binary variable y_j is introduced in the model to represent the selection (or not) of a task (process, technology or equipment) and a binary variable y_i is introduced for the selection (or not) of a resource (material, energy etc.) as follows:

$$y_j = \begin{cases} 1, & \text{if the corresponding task (process, technology or equipment) is selected} \\ 0, & \text{otherwise} \end{cases}$$

$$y_i = \begin{cases} 1, & \text{if the corresponding resource (material, energy etc.) is selected} \\ 0, & \text{otherwise} \end{cases}$$

Then, continuous variables are used to reflect the design and operational decisions that need to be made. For example, the amount of material that is used as input or output of a process, or the amount of material that is consumed during a process are modeled through continuous variables. All the mass and energy characteristics of the tasks that arise from the mass and energy balances are governed by linear relationships with respect to the inputs/outputs and conversion rates.

The various constraints that govern a FSC are also captured through the introduction of equality and inequality constraints. Typically, these constraints are imposed by the conservation of mass or energy (mass and energy balances) within the supply chain, the conversion rates of a task/process, raw material availability, and/or capacity and technological limitations. For example, limited supply of resources for a production process leads to constraints derived from the relationship between this supply and its possible utilization by different tasks. Constraints may be also introduced from externalities such as governmental policies, market restrictions etc., in a form of limitations in the supply of resources and/or demand of products. Finally, big-M constraints are used to ensure that a process is not operational unless it is built. If it is built, then certain limitations are enforced to the model e.g. operating levels of a process may not exceed an upper bound of M.

The existence of both continuous and integer variables in approximated linear forms lead to the formulation of the FSC model as a mixed-integer linear programming (MILP) problem. The performance criterion is denoted as objective function, and can involve economic, energy efficiency and/or environmental features. Here, the objective functions are matched with the aforementioned goals and characteristics of CE as can be seen in Table 1. Therefore, the reduction of material losses and residuals is explored through the minimization of the generated waste, and the like. In case non-linear terms are required either in the objective function and/or in the constraints to represent the involved phenomena, then the model is classified as mixed-integer nonlinear programming (MINLP) problem. This implies a number of difficulties associated with the modeling and the solution of such problems, which must be carefully addressed (Floudas, 1995; Floudas, 2013), and are beyond the scope of the proposed framework.

2.5. Step 5: Single or multi-objective optimization and assessment

The final step of the CE-FSC framework involves the optimization of the model developed in the previous steps, considering single or multi-objectives. In case of a single objective, the optimal solution is easily determined against other solutions by comparing their objective function values. When more than one objective function is involved and must be optimized systematically and simultaneously, then the problem is called multi-objective optimization. In general, there is no single global solution for this type of problems but rather a set of solutions that define the best trade-off among the competing objectives. The set of these non-dominated solutions over the entire feasible space is called pareto-

Table 1
Formulating the objective functions based on the CE goals.

#	CE goals & key characteristics	Objective functions
1	Reduction of material losses/residuals: Waste and pollutants minimization through the recovery and recycle of materials and products.	↔ Minimization of generated waste, Maximization of recycling
2	Reduction of input and use of natural resources: The reduction of the stresses posed on natural resources through the efficient use of natural resources.	↔ Minimization of consumed raw materials and natural resources
3	Increase in the share of renewable resources and energy: Replacement of non-renewable resources with renewable ones, limiting the use of virgin materials.	↔ Maximization of total energy and/or renewable energy output
4	Reduction of emission levels: The reduction in direct and indirect emissions/pollutants.	↔ Minimization of GHG emissions
5	Increase the value durability of products: Extension of product lifetime through the redesign of products and high-quality recycling.	↔ Maximization of product, equipment and packaging durability

optimal set, and a pareto efficient front is generated from the boundary of this set.

The most commonly used methods for solving multi-objective optimization problems are the weighted sum method and the ε -constraint method (Ehrgott, 2006; Mavrotas, 2009). In the first method, the multi-objective problem is transformed into a single objective one by adding weighted objectives. The weights used reflect the relative importance of each objective. The second method involves the optimization of one of the objective functions using the rest of the objective functions as constraints of the problem (Chankong & Haimes, 2008; Liu et al., 2010; Pappas et al., 2021). In the developed CE-FSC framework the ε -constraint method is used, ensuring that the pareto solutions are evenly distributed over the solution space, while attaining a precise representation of the efficient set. The user can even specify the number of the generated efficient solutions by adjusting the number of intervals on the feasible region.

3. Case study: Circular Economy supply chain of coffee

In this section, the supply chain of coffee is selected for demonstrating the applicability and effectiveness of the proposed CE-FSC framework, as a tool for designing and optimizing the transition from the current linear supply chain of coffee to a circular one. Coffee has been selected here since it is one of the most popular beverages globally with more than 167 million 60-kg bags of coffee being consumed yearly worldwide (Baratsas et al., 2021b). This is translated into over 2 billion cups of coffee being consumed on daily basis (ICO, 2020; Lombardini, 2017). As a result, the global coffee supply chain creates an estimated 23 million tons of organic coffee waste per year (Pauli, 2010), while it requires a considerable amount of resources such as energy and water. Coffee industry has also an enormous impact in the economy, representing approximately 1.6% of the total U.S GDP (USA, N.C.A, 2015). Therefore, such as global supply chain that produces a lot of waste and uses a lot of resources, is ideal for the demonstration and application of the proposed framework towards CE.

A typical coffee supply chain is shown in Fig. 3. Coffee cherries are harvested and then processed in two different ways, the dry and the wet process, resulting in different coffee products and by-products as well as products of different quality. In the dry process, the cherries are dried for a period up to three weeks (i.e. Drying) and then the outer and the inner shells are mechanically removed (i.e. Hulling), producing the desirable green coffee beans along with the husk as a by-product (Ullmann, 2012). Conversely, the wet process requires excessive amount of water and is conducted in multiple stages. The process start with the removal of the outer skin that covers the beans (i.e. Pulping), and then continues with the complete removal of the mucilage from the parchment (i.e. Fermentation & Washing). Then, the parchment is dried either naturally under the sun or technically in a dryer (i.e. Drying) until its moisture level reaches about 10%. Finally, the parchment is removed mechanically (i.e. Peeling & Polishing), producing the desirable green coffee beans (Ghosh & Venkatachalapathy, 2014; Murthy & Naidu, 2012b; Ullmann, 2012). Green coffee beans require further processing before become available for consumption. As such, the green coffee beans must be roasted (i.e. Roasting), acquiring a characteristic flavor and aroma, and becoming available for consumption as whole beans. The roasted coffee is then grounded and can be consumed either as a brew beverage (i.e. Coffee Beverage), after brewing, or further treated by extraction, evaporation/concentration, and drying and consumed as Soluble/Instant Coffee (Ullmann, 2012). Caffeine is responsible for the stimulating effect of coffee, and so decaffeination is an extra step that must be taken before roasting the green coffee beans, so as to remove caffeine from the beans.

Apart from the desirable products, wastes and by-products, namely, husk, pulp, mucilage, parchment, silverskin etc. are generated during the coffee supply chain, while significant amounts of resources such as energy and water are also consumed. The overall life cycle burdens of

even just one cup of spray dried soluble coffee, equivalent to 4.44 g of green coffee, are significant, with approximately 1 MJ of primary non-renewable energy and up to 400 ltr of water consumed, 70 g of CO₂eq released (Humbert et al., 2009), 3 g of spent coffee and 12 g of coffee by products (pulp, mucilage, parchment) generated (Murthy & Naidu, 2012b). Moreover, plastics are used in various stages of the coffee supply chain introducing another substantial environmental burden.

With the current linear supply chain model (see Supplementary Fig. 1), only a small fraction of these burdens are reused or recycled even though there are plenty of studies demonstrating sustainable alternatives (Blinová et al., 2017; Chala et al., 2018; Murthy & Naidu, 2012b). Hence, as the coffee consumption increases, so does the amount of organic coffee waste and the amount of resources used, aggravating both the waste, water and energy management problems.

A solution to this problem would be the transition to a circular supply chain (see Supplementary Fig. 2), where renewable energy resources and more efficient processes will be utilized; water consumption will be reduced and wastewater treatment will be applied; waste generation will be minimized, and all wastes will be collected and utilized for the production of alternative products. The material flows ultimately shall be closed, while the energy flows shall be opened. However, it is evident that the transition to a CE model while tackling the challenges from the multi-scale and multi-faceted coffee supply chain require a holistic systems engineering approach. Therefore, the proposed CE-FSC framework can be utilized in this direction, ensuring an effective and efficient transition. The following sections demonstrate step by step the application of the framework in the supply chain of coffee.

3.1. Step 1: Production & processing pathways

As an initial step, the coffee supply chain is modeled by identifying the inputs and outputs along with the processes that take place so as to produce the desirable end-products. In this supply chain, three are the desirable end-products i.e. the whole beans, the coffee beverages and the soluble/instant coffee (Fig. 3), while coffee cherries and water are considered as the main inputs. Moreover, the alternative pathways for the production of the desired product have to be identified and assessed, i.e. wet or dry method for the production of green beans (Chala et al., 2018), decaffeinated or caffeinated coffee. As it is shown in the following steps, the selected pathway(s) might be different each time, depending on the objective(s) of the optimization problem. This complexity requires extra care during the modeling process.

3.2. Step 2: Waste, loss & by-products valorization pathways

As a second step, the waste, losses and by-products of the coffee supply chain must be identified. Coffee husk is the main pre-roasting by-product from the dry processing method, while coffee pulp, mucilage and parchment are the by-products of the wet processing method. Silver skin is the by-product from roasting the green beans, and spent coffee grounds (SCG) are the final by-products from either brewing or extraction processes. The majority of the wastewater is generated during pulping and fermentation. Thus, a waste waste-treatment facility is considered so as to properly treat this water either for re-use in the coffee supply chain or for safe discharge back to the environment. Similarly, to the previous step, the alternative pathways for the valorization of the wastes have to be identified and assessed. Thus, an extensive literature review shall be conducted. The following tables highlight such alternative pathways for the valorization of the coffee wastes and by-products for the production of energy (Table 2a), as well as for the production of value added products (Table 2b). This analysis, in conjunction with feedback from experimentalists, can help towards the identification of sustainable CE coffee supply chain alternatives.

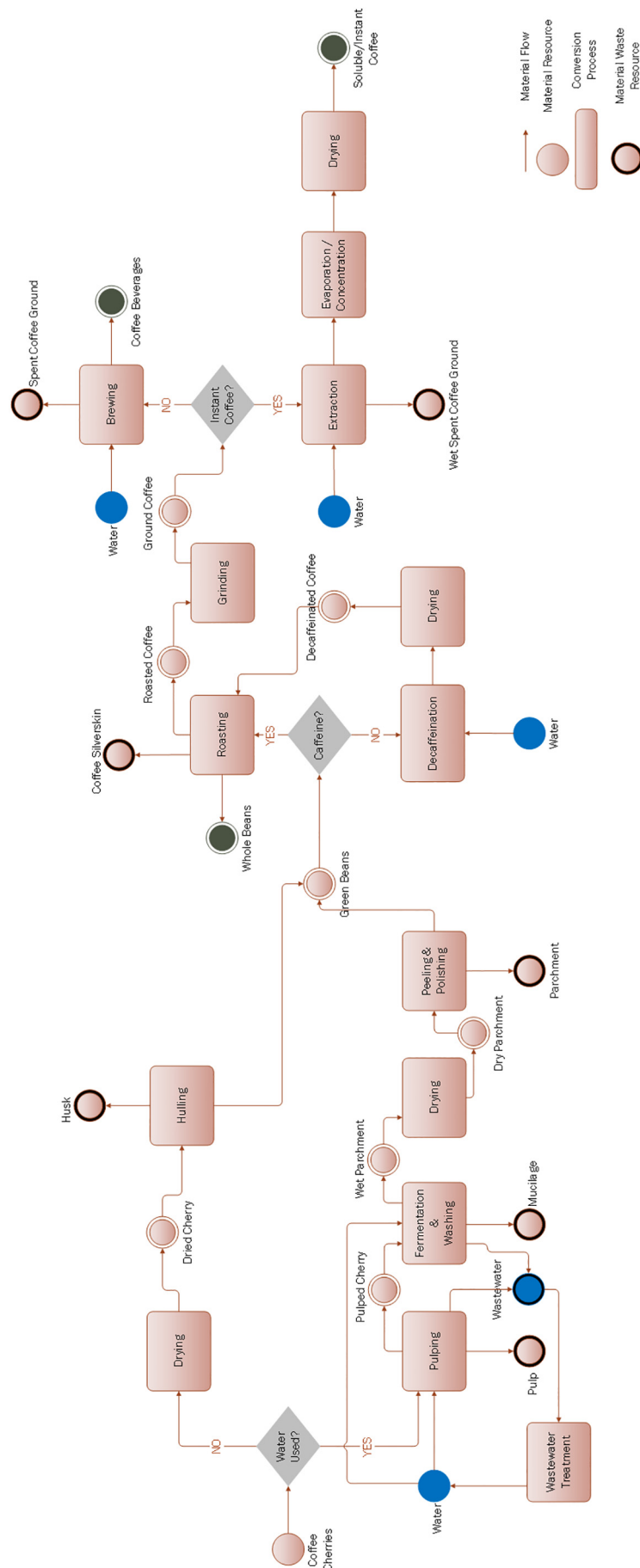


Fig. 3. Supply chain of coffee.

Table 2a

Valorization of coffee by-products & wastes for the production of bio-energy.

Coffee by-products & wastes	Bio-energy production						
	Biodiesel	Bioethanol	Biogas	Bio-oil	Fatty acid methyl ester (FAME)	Fuel pellet	Hydrogen
Coffee husk		Gouvea et al., 2009	Blinová et al., 2017 Chala et al., 2018 Murthy & Naidu, 2012b Ulsido et al., 2016			Blinová et al., 2017	
Coffee pulp		Blinová et al., 2017 Gurram et al., 2016	Blinová et al., 2017 Chala et al., 2018 Figueroa et al., 2016			Blinová et al., 2017	
Coffee mucilage		Orrego et al., 2018	Chala et al., 2018				Hernández et al., 2014
Coffee parchment							
Coffee silverskin		Blinová et al., 2017 Figueroa et al., 2016					
Spent coffee grounds	Blinová et al., 2017 Campos-Vega et al., 2015 Banu et al., 2020 Karmee, 2018 Murthy & Naidu, 2012b Kwon et al., 2013 Tongcumpou et al., 2019 Berhe et al., 2013 Haile, 2014, Vardon et al., 2013, McNutt et al., 2019	Blinová et al., 2017 Banu et al., 2020 Karmee, 2018 Figueroa et al., 2016 Murthy & Naidu, 2012b Kwon et al., 2013 McNutt et al., 2019	Banu et al., 2020 Karmee, 2018 Figueroa et al., 2016 Li et al., 2014 Lee et al., 2019 Vitřz et al., 2016	Banu et al., 2020 Karmee, 2018 Figueroa et al., 2016 Li et al., 2014 Vardon et al., 2013	Banu et al., 2020 Karmee, 2018 Lee et al., 2019	Blinová et al., 2017 Banu et al., 2020 Karmee, 2018 Figueroa et al., 2016 Stylianou et al., 2018 Haile, 2014	Banu et al., 2020 Karmee, 2018

3.3. Step 3: Resource-Task-Network (RTN)

In the previous steps the main and alternative pathways of the coffee supply chain have been identified, and so the next step involves the generation of a Resource-Task-Network (RTN) representation that incorporates all these pathways. Here, and for demonstrating purposes, only the alternative pathways for the production of bio-energy are considered. Fig. 4 illustrates the developed RTN representation of the supply chain of coffee, capturing the sections in the production as well as in the consumption countries, the conversion coefficients of the various processes, along with waste valorization alternatives for the production of energy.

The part of the supply chain from the plantation of the coffee cherries, to the production of green coffee beans through the dry or wet processing methods, typically takes place in the production countries, while the rest of the supply chain, that includes the production of the final products, takes place in the consuming countries. The coffee producing countries consume significant resources in the form of raw materials, energy, and water while the generated wastes and by-products constitute a source of severe contamination and environmental threat. The consuming countries face similar problems, with the most challenging being related with the waste management of the coffee by-products and wastes.

The conversion coefficients of the various processes are another crucial factor within the coffee supply chain. On average, just 190 kg of green coffee are produced per ton of coffee cherries (Ghosh & Venkatachalapathy, 2014; Mutua, 2000; Ulsido et al., 2016), due to the mass reduction that occurs during the drying process as a result of the high moisture of coffee beans, along with the considerable waste that is generated during the dry or wet processes (Braham & Bressani, 1979; Gathuo et al., 1991). Moreover, on average one ton of green coffee generates 370 kg of coffee beverages or 370 kg of soluble/instant coffee (ICO, 2011; ITC, 2021), and about 650 kg of SCG or about 2 kg of wet SCG from each kg of soluble/instant coffee produced (Banu et al., 2020; Dugmore, 2014; Murthy & Naidu, 2012b).

About 23 kg of CO₂eq per ton coffee cherries and 76 kg of CO₂eq per ton coffee cherries are released during the dry and wet processes respectively, while substantial is also the environmental burden during the brewing and extraction processes, with 1.38 ton of CO₂eq per ton of roasted coffee and 3.28 ton of CO₂eq per ton of roasted coffee

respectively (Humbert et al., 2009). It is worth mentioning, that no CO₂ emissions are released to the atmosphere during any of the waste valorization processes. Similarly, wet method requires substantial more power consumption (2.735 MWh per ton of coffee cherries) in comparison to the dry method (0.103 MWh per ton of coffee cherries). Minimal is the energy requirement for the roasting process (0.042 MWh per ton of green coffee) (Morawicki & Hager, 2014), while coffee extraction process (Morawicki & Hager, 2014) is more energy intensive (4.68 MWh/ton instant coffee) than brewing process (1.87 MWh/ton coffee beverages) (Humbert et al., 2009). Finally, the water conversion coefficients are estimated based on (Chapagain & Hoekstra, 2003), with 10.5 cubic meters of water per ton of roasted coffee been used during brewing process, and 11.67 cubic meters of water per ton of roasted coffee been used during the extraction process. As expected, zero water is consumed during the dry process, while 9.7 cubic meters of water per ton of coffee cherries is consumed during the wet process.

3.4. Step 4: Mixed-Integer Linear Programming (MILP) model

First, all available types of resources I , including material and energy resources, as well as all available types of tasks J , including the primary coffee production processes, the waste valorization and the waste treatment processes, are denoted as follows:

$$I = \{i_1, i_2, \dots, i_{|I|}\},$$

and

$$J = \{j_1, j_2, \dots, j_{|J|}\}$$

Also, the following subsets are denoted:

$$\begin{aligned} I^{WS} & \text{ waste resources, } i \in I^{WS} \\ I^{WT} & \text{ water resources, } i \in I^{WT} \end{aligned}$$

Then, the resource and task parameters are defined. The supply and demand of the various resources form the resource parameters, while the conversion coefficients of the various processes, along with the

Table 2b
Valorization of coffee by-products & wastes for the production of value-added products.

Coffee by-products & wastes	Value-added product recovery					Caffeine	Carbon Material	Composting	Enzymes	Food ingredients
	Antioxidants	Biochar	Biopigments	Biopolymers	Biosorbents					
Coffee husk				Figuerola et al., 2016	Blinová et al., 2017	Esquivel & Jiménez, 2012		Blinová et al., 2017 Figuerola et al., 2016 Murthy & Naidu, 2012b	Murthy & Naidu, 2012b Murthy & Naidu, 2012a	Blinová et al., 2017 Figuerola et al., 2016 Murthy & Naidu, 2012b
Coffee pulp				Murthy & Naidu, 2012b Esquivel & Jiménez, 2012	Murthy & Naidu, 2012b	Esquivel & Jiménez, 2012		Blinová et al., 2017 Murthy & Naidu, 2012b	Blinová et al., 2017 Murthy & Naidu, 2012b	Blinová et al., 2017 Murthy & Naidu, 2012b
Coffee mucilage										
Coffee parchment	Figuerola et al., 2016					Esquivel & Jiménez, 2012		Esquivel & Jiménez, 2012		Blinová et al., 2017
Coffee Silverskin	Rodrigues et al., 2015									
Spent Coffee Grounds	Blinová et al., 2017 Campos-Vega et al., 2015 Banu et al., 2020 Karmee, 2018 Figuerola et al., 2016 Murthy & Naidu, 2012b Tongcumpou et al., 2019 Pettinato et al., 2019 Esquivel & Jiménez, 2012 McNutt et al., 2019	Banu et al., 2020 Karmee, 2018 Stylianou et al., 2018 Li et al., 2014 Tongcumpou et al., 2019 Vardon et al., 2013	Campos-Vega et al., 2015 Banu et al., 2020 Karmee, 2018 Figuerola et al., 2016	Blinová et al., 2017 Campos-Vega et al., 2015 Banu et al., 2020 Karmee, 2018 Figuerola et al., 2016 Murthy & Naidu, 2012b Stylianou et al., 2018	Blinová et al., 2017 Banu et al., 2020 Karmee, 2018 Figuerola et al., 2016 Murthy & Naidu, 2012b	Esquivel & Jiménez, 2012 Campos-Vega et al., 2015 Banu et al., 2020	Campos-Vega et al., 2015 Banu et al., 2020 Karmee, 2018 Murthy & Naidu, 2012b	Blinová et al., 2017 Campos-Vega et al., 2015 Figuerola et al., 2016 Stylianou et al., 2018 McNutt et al., 2019	Stylianou et al., 2018	Blinová et al., 2017 Campos-Vega et al., 2015 Karmee, 2018 Murthy & Naidu, 2012b Stylianou et al., 2018

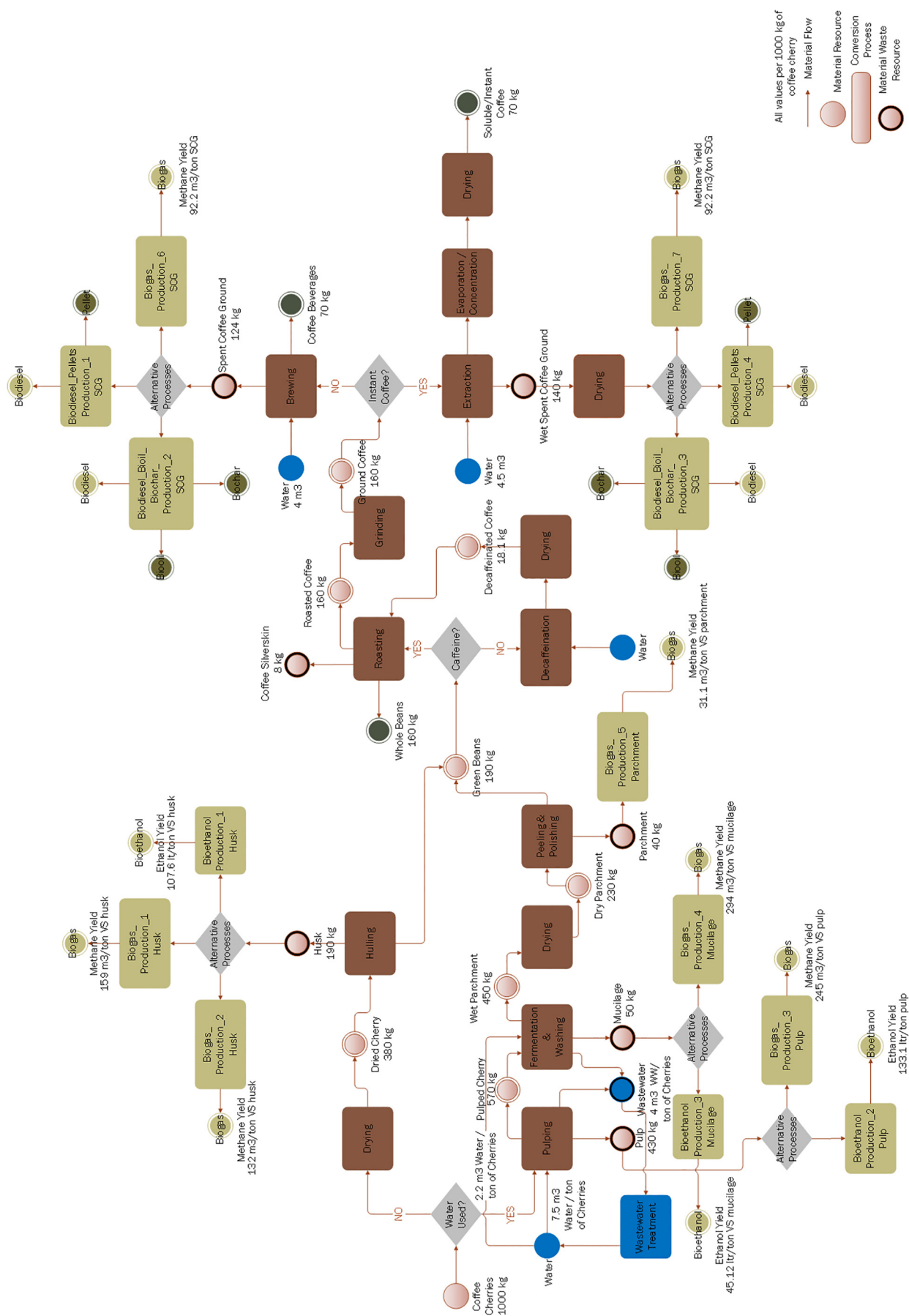


Fig. 4. RTN of coffee supply chain.

CO₂ emissions coefficients and the energy consumption or generation coefficients form the process parameters. In particular,

- sup_i resource supply parameter, $i \in I$
- dem_i resource demand parameter, $i \in I$
- $pc_{i,j}$ process conversion coefficient, $i \in I$, and $j \in \mathcal{J}$
- $co2_j$ CO₂ conversion coefficient, $j \in \mathcal{J}$
- pw_j energy conversion coefficient, $j \in \mathcal{J}$
- l_{supi} lower bound of supply resource i
- u_{supi} upper bound of supply resource i
- l_{demi} lower bound of demand resource i
- u_{demi} upper bound of demand resource i

Moreover, the design and operational decisions are governed by the following positive variables:

- p_i amount of resource i purchased or supplied, $\forall i \in I \{l_{supi} \leq p_i \leq u_{supi}\}$
- s_i amount of resource i sold or demanded, $\forall i \in I \{l_{demi} \leq s_i \leq u_{demi}\}$
- x_j production level of task j , $\forall j \in \mathcal{J} \{0 \leq x_j \leq \infty\}$

Finally, the selection or not of a process is governed by the following binary variable:

- y_j 1 if the corresponding task is selected, 0 otherwise, $\forall j \in \mathcal{J} \{0 \leq y_j \leq 1\}$

The following two equations express the constraints that govern the coffee supply chain. Eq. (1) represents the total mass balance of the coffee supply chain. For any resource i in the model, the amount of resource purchased or supplied (i) plus the amount of resource produced or consumed by the tasks j , ($\sum_{j \in \mathcal{J}} pc_{ij} \cdot x_j$) must be equal to the amount of resource sold or demanded (S_i).

$$p_i + \sum_{j \in \mathcal{J}} pc_{ij} \cdot x_j = s_i \quad \forall i \in I \quad (1)$$

Eq. (2) represents the big-M constraint for the production level of task j . The coefficient M introduces a very large number in the equation, which actually dictates specific outcomes or limitations to the model e.g. a task is selected only if it is built, and then an upper bound M is enforced to the production level of this task.

$$x_j \leq M \cdot y_j \quad \forall j \in \mathcal{J} \quad (2)$$

3.5. Step 5: Single or multi-objective optimization and assessment

The final step involves a multi-objective optimization strategy to obtain trade-offs among multiple CE objectives, such as maximizing the energy output while minimizing the coffee cherries consumption, under different demand scenarios for the final products i.e. coffee beverages, instant coffee and whole beans, while considering the subject constraints. A variety of single or multi-objective functions can be optimized depending on the scenario under consideration. For the design of a CE-FSC, and as is discussed in Section 2.4 and presented in Table 1, the objective functions are matched with the CE goals and key characteristics.

Therefore, by looking to increase the share of the renewable resources and energy, the energy output of the supply chain (CEO) is maximized, while by looking to reduce the input, the coffee cherries consumption (CCC) is minimized. Likewise, by targeting the reduction of natural resources, the consumption of water (CWC) is minimized, while the reduction of material losses and emission levels will be achieved through minimizing the waste generation (CWG) and the CO₂ emissions (CEM) respectively.

Eqs. (3)–(7), contemplate the goals of CE-FSC as five different single objective functions.

$$\begin{aligned} \text{Objective 1 :} \quad & \min \text{ CWG} = \min \sum_{i \in I^{WS}} s_i \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (3)$$

$$\begin{aligned} \text{Objective 2 :} \quad & \min \text{ CCC} = \min p_{cherries} \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (4)$$

$$\begin{aligned} \text{Objective 3 :} \quad & \min \text{ CWC} = \min \sum_{i \in I^{WT}} p_i \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (5)$$

$$\begin{aligned} \text{Objective 4 :} \quad & \max \text{ CEO} = \max \sum_{j \in \mathcal{J}} pw_j \cdot x_j \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (6)$$

$$\begin{aligned} \text{Objective 5 :} \quad & \min \text{ CEM} = \min \sum_{j \in \mathcal{J}} co2_j \cdot x_j \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (7)$$

Eqs. (8)–(12) contemplate the same CE goals, but this time simultaneously as a multi-objective optimization problem. For example, Eq. (8) describes the minimization of coffee cherries consumption, while maximizing the total energy output.

$$\begin{aligned} \text{Multi-Objective 1 :} \quad & \min \text{ CCC} \quad \& \quad \max \text{ CEO} \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (8)$$

$$\begin{aligned} \text{Multi-Objective 2 :} \quad & \min \text{ CCC} \quad \& \quad \min \text{ CWG} \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (9)$$

$$\begin{aligned} \text{Multi-Objective 3 :} \quad & \min \text{ CWG} \quad \& \quad \max \text{ CEO} \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (10)$$

$$\begin{aligned} \text{Multi-Objective 4 :} \quad & \min \text{ CWC} \quad \& \quad \max \text{ CEO} \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (11)$$

$$\begin{aligned} \text{Multi-Objective 5 :} \quad & \min \text{ CEM} \quad \& \quad \max \text{ CEO} \\ \text{s.t.} \quad & \text{Eqs. (1)–(2)} \end{aligned} \quad (12)$$

The multi-objective optimization problems are solved using the ε -constraint method (Ehrgott, 2006; Mavrotas, 2009), which converts the multi-objective optimization problem to a series of single-objective optimization sub-problems. As an example, for solving multi-objective problem 1, the first step requires the solution of the problem using only one objective function f_1 , in this case described by Eq. 4. This leads to an optimal solution, denoted as x_1^* . The minimum of the second objective function f_2 (Eq. (6)) is obtained at this optimal point x_1^* , since any value lower than this for f_2 will not increase the value of f_1 . Hence, the minimum of f_2 is denoted as $\theta^L = f_2(x_1^*)$.

The next step involves the solution of another optimization problem, this time with only the other objective function f_2 , as it is described by Eq. (6). Similarly, another optimal solution is obtained, denoted as x_2^* , which is the maximum of f_2 , so it is denoted as $\theta^U = f_2(x_2^*)$. Thus, the feasible region of f_2 is defined as $[\theta^L, \theta^U]$. This region is divided equally into N intervals, and so $\theta \in [\theta^L, \theta^U]$. Hence, the original multi-objective problem can be converted into the following single objective optimization problems:

$$\begin{aligned} \min \quad & \text{CCC} \\ \text{s.t.} \quad & \text{CEO} \geq \theta \\ & \text{Eqs. (1)–(2)} \end{aligned} \quad (13)$$

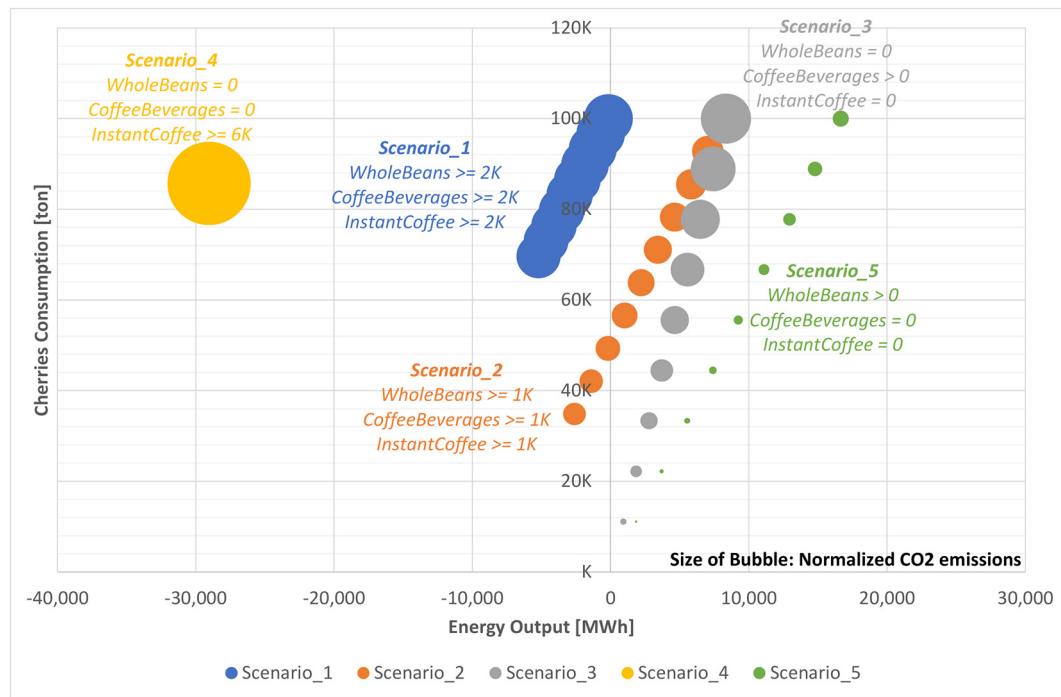


Fig. 5. Pareto analysis for problem 1: max energy output & min cherries consumption & normalized CO₂ emissions.

4. Results and discussion

The CE-FSC mixed-integer optimization model is implemented in Python and solved utilizing Gurobi V9.0.2 default solver (Gurobi Optimization, 2020) on an Intel 3.5GHz Quad-Core i7 Processor with 16 GB of RAM. For the multi-objective function problems (Eqs. (8)–(12)) under one scenario, the model features 138 equations, 58 continuous variables, and 18 binary variables, and the average time to solve it is 0.01 s.

Five different scenarios for the supply of coffee cherries and the demand of final coffee products are investigated for each of the single or multi-objective optimization problems. They are chosen so as to demonstrate the applicability and effectiveness of the framework in conducting quantitative analysis of any food supply chain under circular economy considerations while capturing even the most extreme cases. The supply and the demand values are arbitrarily selected for illustration purposes. For easy comparison, the maximum supply of coffee cherries stays the same among the scenarios at 100,000 tons. For scenarios 1 and 2, the demand for the three final products is set at 2000 tons and 1000 tons respectively. Scenario 3 involves only demand for coffee beverages without any demand for the other two products. Similarly, scenario 5 involves only demand for whole beans without any demand for the other two products. Finally, the demand for instant coffee in scenario 4 is set higher or equal to 6000 ton with zero demands for the other two products. Scenario 4 requires a specific demand target to be met since the production of instant coffee introduces higher environmental and production burdens in comparison to the other two products, thus under an optimization perspective, there will be no incentives to generate any amount, unless a specific target is set. Please also refer to Supplementary Table 1.

By utilizing the CE-FSC framework that is described in the previous sections, the solution of each single objective optimization problem as well as the pareto fronts of each multi-objective optimization problem are generated. The solutions of the single objective optimization problems are shown in Supplementary Figs. 3 to 7. Here, the results of multi-objective optimization problems 1 (Eq. (8)) and 4 (Eq. (11)) are presented, whereas the results of the rest of the multi-objective

optimization problems are shown in Supplementary Figs. 8 to 10. Supplementary Figs. 11 and 12 expand the results of the trade-off analysis for the multi-objective optimization problems 1 and 3 respectively, by incorporating three different values (low: 0.1034, average: 0.7281 (+604%), high: 1.3528 (+1208%), unit: MWh/ton coffee cherries) for the parameters related to the drying process (ICO, 2021; Morawicki & Hager, 2014).

Fig. 5 reveals the results of such a trade-off analysis for the multi-objective problem 1 of minimizing the coffee cherries consumption while maximizing the total energy output (minCCC & maxCEO), subject to the constraints of the coffee supply chain which are described by Eqs. (1)–(2). The colors in Fig. 5 represent different demand scenarios for the final products. The low values of the parameters in the drying process are used. Since this is a multi-objective optimization problem, a pareto of solutions is generated and each bubble demonstrates a different optimal solution from the pareto. An optimal solution refers to the selection of specific values for the binary and continuous variables so that the imposed constraints are satisfied and the objective functions are optimized. Practically, each bubble represents a specific operational profile of the coffee supply chain, while the size of a bubble depicts the normalized CO₂ emissions (min-max normalization). As it is also discussed in Section 2.5, the ϵ -constraint method is used for the solution of the multi-objective optimization problem. The pareto solutions for each demand scenario, meaning the bubbles with the same color, are evenly distributed over the solution space and here the number of generated efficient solutions has been specified to 10.

An upper bound of available cherries has been set at 100,000 tons for all 5 scenarios. Scenarios 1 and 2 require certain demands to be met for all 3 final products. As expected, the higher the consumption of cherries, the higher the energy produced. Once the target demands are met, the excessive amount of cherries is converted to whole beans, while the excessive amount of coffee by-product is used to produce more energy. This is because even though whole beans can be sold as a final product to the market, they require further processing, either brewing or extraction, so as to yield the end coffee drink. Thus, producing just whole beans is favorable in terms of energy and environmental footprint.

The operating profiles of scenario 1 (with higher energy demands) are more to the left on the graph than those of scenario 2, because the extra demand of coffee beverages and instant coffee requires more brewing and extraction, which are both energy intensive processes. The rest of the scenarios represent instances where the demand of only one final product is specified. In particular, scenario 5, even rather unrealistic since it refers exclusively to demand of whole beans and requires further processing to produce the coffee drinks, it demonstrates the best-case scenario in terms of both energy and environmental performance. On the contrary, scenario 4, with only instant coffee as a deliverable, is the worst-case scenario both in terms of energy and environmental efficiency. Just one operating profile is produced since the optimal solution for both objectives refers merely to the satisfaction of demand. Finally, in scenario 3 that describes the case of demand solely coming from coffee beverages, the operating profiles demonstrate a steeper slope in comparison to the ones from the other scenarios. This behavior is attributed to the different energy and environmental benefits that coffee beverages have in comparison to the other coffee products. Supplementary Fig. 11 and 12 highlight the effects uncertain parameters related to the drying process have on the multi-objective optimization process. As the values of drying parameters increase, the optimal solutions require more energy to meet the demand scenarios.

The second trade-off analysis is highlighted in Fig. 6 for the multi-objective problem 4 of minimizing the water consumption while maximizing the total energy output (min CWC & max CEO), subject to the constraints of the coffee supply which are described by Eqs. (1)–(2). Similarly to the previous problem, every color in Fig. 6 represents a different demand scenario for the final products, while the size of the bubbles represents the CO₂ emissions. Likewise, the ε -constraint method is utilized to solve this multi-objective problem, resulting in the generation of a pareto of solutions. The maximum supply of coffee cherries has been bounded to 100,000 ton.

In Scenarios 1 and 2, the demand of coffee beverages and instant coffee are just met and the excess is converted in whole beans because this is environmentally preferable. On the contrary, scenario 3 produces up to 7000 ton of coffee beverages, because the consumption of more coffee beverages results into more spent coffee, which ultimately results

in more energy generation. However, the trade-off between energy output and water consumption is clear in this scenario, since an increase in energy output of just over 7000 MWh requires the consumption of more than 155,000 ton of water. Thus, the user is able to select its operational profile considering the environmental effects. An interesting case is revealed in scenario 4, where the optimal solution is reached once the demand is met, since it is not beneficial neither in terms of energy nor in terms of water to produce more instant coffee. This scenario also, demonstrates the higher burden with respect to CO₂ emissions. Lastly, in scenario 5, even though no water is consumed, the production reaches 17,000 tons of whole beans. The produced energy is generated from the waste of husk, as a result of the dry processing method, however and as it is mentioned before, this scenario is rather unrealistic since further processing is required for the production of the end coffee drinks. In this multi-objective optimization problem, a pareto with distinct optimal solutions is generated only for scenario 3. For the rest of the scenarios, there is only one optimal solution that satisfies the subject constraints, resulting in just one bubble for each scenario.

Future developments on the illustrative case study of the coffee supply chain could include valorization pathways for the utilization of wastes and by-products for the production of high added value products. Scaling issues from the laboratory and proof of concept levels to the full scale and product release levels must be always taken into consideration. Hence, analytical process design and synthesis along with feedback from experimentalists are crucial. The model approximations could be also revisited, and high-fidelity models can be developed for proper testing. The rising number of alternatives would require the development and implementation of holistic assessment CE indicators and metrics. Our group is currently working in the development of such a CE assessment methodology (Baratsas et al., 2021a), which will be combined with the current CE-FSC framework for the selection of the most “circular” pathways. These steps would be obviously applicable to any FSC under examination with CE considerations. Validation strategies through energy systems engineering optimization approach will be also required for the efficient design and operation of the most promising processes.

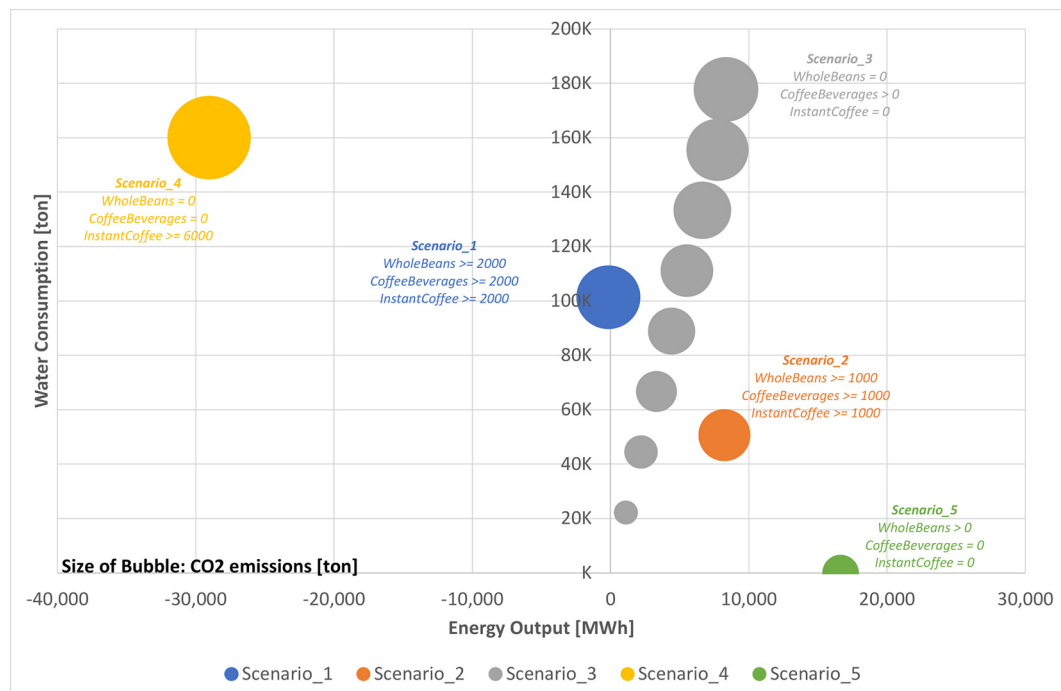


Fig. 6. Pareto analysis for problem 4: max energy output & min water consumption & CO₂ emissions.

5. Conclusions

The dissemination and implementation of CE is fundamental for the fruition of the social, environmental and economic benefits of the 2030 Agenda and the Paris Agreement, along with the sustainable recovery from COVID-19. This paper presents a system engineering framework and decision-making tool for the analysis and trade-off modeling and optimization of interconnected FSCs considering the principles and goals of CE. It aims to provide a holistic quantitative tool that assists towards the transition to CE-FSCs by efficiently tackling the plethora of newly introduced challenges. This is achieved through the modeling and systematic integration of recent technological, experimental, academic and industrial knowledge in the design and operation of FSCs using a RTN superstructure representation. The resulting MILP model incorporates all the unique characteristics of the FSC network, any constraints along with all the alternative production, processing and valorization pathways, and is optimized under single or multi-objective CE criteria. Since CE introduces conflicting or competing objectives, the multi-objective optimality is critical, and is implemented through the generation of the pareto optimal set over the entire feasible space.

The developed framework contributes to the literature by explicitly incorporating all CE goals and objectives into the design and operation of FSCs. It also serves a dual role, since it does not only allow the identification and selection of the optimal tasks from the list of alternatives under specific CE objectives, but also enables the identification of any potential bottlenecks. This feature promotes the research and development of certain, less efficient parts of the supply chain. The framework is also flexible since the set of resources and the corresponding available supply of inputs as well as the target demands of the final products can be constantly updated, reflecting new trends and developments. It can be also utilized from users with different backgrounds and considerations. Academics and experimentalists could focus more on the improvement of existing tasks, or the creation of completely new ones, private corporations could focus on optimizing their entire FSCs through the lens of CE holistically, and finally governmental policymakers could quantitatively identify areas that require funding and/or specific legislative actions.

The supply chain of coffee has been selected as an indicative case study for demonstrating the unique features of the proposed framework. In particular, the effectiveness and the applicability of the framework in transforming the linear supply chain to a circular one while analyzing different supply and demand scenarios, under CE objectives simultaneously is demonstrated. Since the objectives of CE and its stakeholders are usually competing, a multi-objective optimization approach is utilized. The computational results prove that the MILP problem can be optimally solved, producing different pareto fronts depending on the CE objectives. Therefore, it can be used as a decision-making tool that captures all the potential sets of resources and tasks under any design and operational criteria and/or external conditions.

The proposed framework can be utilized in other food supply chains, ensuring their effective transition towards circularity. Moreover, extra constraints in the modeling can be introduced to capture inherent characteristics of FSCs systematically, such as perishability and quality decay of dairy, meat-poultry, vegetable products. The identification of valorization techniques to eliminate wastes and produce new valuable products along with the ability to simulate different demand and supply scenarios provide a powerful tool towards circularity. Future work may expand into other classes of problems, including phenomena, objective functions and/or constraints with non-linear terms, thus resulting into mixed-integer nonlinear programming (MINLP) problems. In addition, uncertainty issues related to system's externalities or inherent characteristics such as weather conditions, consumer preferences, demand and supply fluctuations and so on (Avraamidou & Pistikopoulos, 2017; van der Vorst et al., 1998), can be also taken into consideration in future work by incorporating sensitivity analysis, parametric optimization, stochastic

and robust optimization into the framework (Avraamidou & Pistikopoulos, 2020; Christopher Frey & Patil, 2002; Zhou et al., 2013). Finally, the current framework considers a central planner deciding for the entire supply chain. Future work would involve the decomposition of the supply chain into its different stakeholders, resulting into multi-agent optimization formulations, and requiring other optimization approaches for its solution (Avraamidou and Pistikopoulos, 2019a,b).

CRediT authorship contribution statement

Stefanos G. Baratsas: Methodology, Software, Validation, Formal analysis, Data curation, Writing – original draft, Writing – review & editing, Visualization. **Efstathios N. Pistikopoulos:** Conceptualization, Methodology, Formal analysis, Writing – review & editing, Supervision, Project administration, Funding acquisition. **Styliani Avraamidou:** Conceptualization, Methodology, Formal analysis, Writing – review & editing, Visualization, Supervision, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.scitotenv.2021.148726>.

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