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| 3 | Non-cooperative game theory to ensure the marketability |
| 4 | of organic fertilizers within a sustainable circular economy |
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- 16 ABSTRACT
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18 To optimize the environmental performance and the conflicting economic interests of the 19 stakeholders that interact within circular integrated waste management systems (CIWMSs), life cycle analysis and game theoretical models - based on the Stackelberg equilibrium - were 20 21 integrated into a multi-objective optimization framework. The framework was used to determine 22 the operational decisions and the configuration of a CIWMS that simultaneously minimize the total 23 global warming impacts (GWI) and maximize the profits of i) the waste managers that valorize the 24 municipal organic waste generated in the Spanish region of Cantabria, and ii) the regional farmers 25 that purchase the organic fertilizers derived from this waste. The resulting bilevel problem was 26 solved applying the Karush-Kuhn-Tucker conditions. The balance between the stakeholders' 27 objectives is reflected in the low prices set for the organic fertilizers (0-2 \in metric ton⁻¹ of compost, 28 and 0-1 €-metric ton⁻¹ of digestate). Although the minimal GWI are constrained by the waste 29 managers' profits, it is possible to push the Pareto frontier toward better outcomes increasing the 30 waste management taxes. The proposed framework proved to be a useful instrument to plan for a 31 sustainable circular economy, warranting that the production and purchase of organic fertilizers is 32 profitable for both ends of the supply chain.

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35 KEYWORDS

- 36 Circular integrated waste management systems
- 37 Organic waste
- 38 Nutrient recovery
- 39 Stackelberg game
- 40 Multi-objective optimization
- 41 Life cycle assessment
- 42 Global warming impacts
- 43 Life Cycle Costing

44 INTRODUCTION

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The economic sector that encompasses agriculture, forestry and other land uses emits almost a quarter of the anthropogenic greenhouse gases.¹ The nitrogen use efficiency of the most cultivated crops is typically below 40%; the remaining nitrogen is released to the atmosphere as $N_2O - a$ powerful greenhouse gas – or leaches into the water bodies causing eutrophication.² Moreover, around 45% of the phosphorus mined worldwide for agricultural purposes ends in the ocean, contributing to eutrophication and the depletion of this non-renewable nutrient.³

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53 On the other hand, solid waste management accounts for about 5% of global warming impacts 54 (GWI).⁴ The diversion of organic waste from landfills prevents the degradation of carbon into CH₄ – 55 a significant contributor to global warming – that occurs under the anaerobic conditions of landfills, 56 and represents an opportunity for nutrient recovery; it has been estimated that the total nitrogen, 57 phosphorus and potassium contained in food, animal and human waste amount to 2.7 times the 58 nutrients processed by the fertilizer industry.⁵

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Finding a common strategy to meet the ever-increasing demand for nutrients and manage organic waste while minimizing the associated environmental impacts and the removal of resources from the environment falls within the scope of a circular economic system. However, a standardized systematic approach to quantify, assess and optimize the performance of a circular economy is still lacking.

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66 Cobo et al.^{6,7} illustrated how process systems engineering can effectively assist decision-makers in 67 this respect by developing a life cycle optimization framework for the sustainable design of Circular 68 Integrated Waste Management Systems (CIWMSs) targeting nutrient circularity. Nonetheless, their 69 study did not consider that an increase in the market share of the fertilizing products recovered 70 from organic waste (hereafter referred to as organic fertilizers) can only be achieved if farmers are 71 willing to purchase these products.

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⁷³ Indeed, the worse performance of organic fertilizers compared with industrial fertilizers – more ⁷⁴ product is required to fertilize the same area $-^{8,9}$ renders them uncompetitive in the absence of ⁷⁵ subsidies. To avert a scenario where waste managers do not get back a return on the investment made in sustainable technologies and accumulate a stock of organic fertilizers that cannot be sold,
trade-offs between their economic interests and those of the farmers must be made. Therefore,
modeling the farmers' response to the prices set for the organic fertilizers is critical to accurately
foresee the behavior of CIWMSs.

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81 Game theory can be applied to optimize the decisions and actions of all the parties involved in a 82 circular supply chain in accordance with their individual – and conflicting – objectives. Nevertheless, few studies have reportedly approached the design of circular systems from a game theoretical 83 84 perspective. Some authors have analyzed the payoff matrices derived from the alternative decisions 85 that the relevant actors within circular systems can make, ¹⁰⁻¹³ whereas others have developed more complex optimization frameworks.¹⁴⁻¹⁶ To the best of the authors' knowledge, the optimization of 86 87 the interactions between the waste managers that valorize municipal organic waste and the farmers 88 that purchase the resulting fertilizing products has not been described in the literature.

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90 Thus, the goal of this paper is to explore how game theory optimization can be used to plan for the 91 implementation of a sustainable circular economy of nutrients by guaranteeing that the production 92 and agricultural application of organic fertilizers is profitable for both ends of the supply chain. This 93 research builds on previous studies that focus on a CIWMS aimed at the valorization of the municipal organic waste generated in the Spanish region of Cantabria.⁷⁻⁹ The results of the study will determine 94 95 the operational decisions and the configuration of the Cantabrian CIWMS that minimize its GWI and 96 optimize the economic performance of the involved stakeholders. Specifically, the research will 97 reveal the types of organic fertilizers that must be produced and the range of prices that should be 98 assigned to them to ensure their acceptance in the market under the restrictions of the case study.

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101 METHODOLOGY

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The integration of life cycle and game theoretical models underpinned the holistic and decentralized
 optimization of the system. The assumptions made and the methodological procedure followed are
 described below.

| 106 | System | model |
|-----|--------|-------|
|-----|--------|-------|

Figure 1 depicts the superstructure containing all the alternative unit processes that could be integrated into the optimal system design. Once the unit processes were separately characterized, the system model was constructed in the GAMS (General Algebraic Modeling System) 28.2.0 optimization platform.¹⁷

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To align this modular modeling approach with the game theoretical model that describes the stakeholders' behavior, the unit processes were split into two subsystems comprising the activities of different groups of agents: the waste management and the agricultural subsystems. The boundaries that delimit the studied CIWMS and the two subsystems are identified in Figure 1.

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118 Regarding the spatiotemporal boundaries of the study, the CIWMS processes the municipal organic 119 waste collected from all the Cantabrian municipalities in one year (83,544 metric ton).¹⁸ The 120 farmers, who purchase the amount of fertilizing products required to grow their crops during that 121 year, are located across the region.

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124 - Life cycle model

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126 An attributional Life Cycle Assessment (LCA) model (based on average data and focusing on the environmentally relevant flows that enter and exit the system)¹⁹ was developed. The functional unit 127 128 was defined as the area that must be annually fertilized to meet the nutrient requirements of the 129 two most cultivated crops in Cantabria – corn and wheat –, which in 2018 occupied 4,118 and 674 ha, respectively.²⁰ The analyzed CIWMS also supplies the electricity generated at the incineration, 130 131 landfill and anaerobic digestion unit processes. To address the system multi-functionality, the direct 132 substitution method was applied, presuming that the electricity generated by the CIWMS replaces 133 the same amount of electricity produced with the average Spanish technology mix.

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The GWI were modeled with the ReCiPe 1.11 method,²¹ considering a 100-year time horizon. The biogenic carbon derived from food waste was quantified as neutral; i.e., it was assumed to have been removed from the atmosphere in the crop production stage.



Figure 1. System boundaries and superstructure

158 The LCA of the individual unit processes that compose the system was carried out with the 159 EASETECH (Environmental Assessment System for Environmental Technologies) 2.3.6 software.²² 160 EASETECH also calculated the composition and flows of the streams exiting each unit process, which 161 served as the input data to the models of the units that further process those streams. The DNDC (Denitrification-Decomposition) 9.5 simulation model²³ was used to predict the mean annual 162 163 fertilization requirements, crop yields, and carbon and nitrogen emissions due to the application of 164 the different fertilizers to the soil in the 100-year timeframe. The DNDC results were transferred to EASETECH to determine the associated GWI. The data required to conduct the LCA, namely the 165 166 waste composition (Appendix A), the life cycle inventories of the waste management unit processes 167 (Appendix B), and the DNDC input data and results (Appendix C) are in the Supporting Information. 168

Life Cycle Costing was used to determine the stakeholders' profits. The economic models of the waste management unit processes were mainly derived from SWOLF (Solid Waste Optimization Lifecycle Framework),²⁴ whereas various sources provided the data to estimate the farmers' profits.²⁵⁻³¹ The selected reference year for the economic data related to the waste management and the agricultural subsystems (Appendix D) is 2015.

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175 It was assumed that the waste managers are free to fix a gate price for the compost and digestate between -10 and 10 € metric ton⁻¹. It is not unusual for European waste managers to pay for the 176 transportation and spreading costs of the organic fertilizers;^{32,33} even negative prices have been 177 178 reported as a measure to incentivize farmers to purchase organic fertilizers.³⁴ The same minimum 179 gate prices were considered for the struvite and $(NH_4)_2SO_4$ produced by subjecting the liquid 180 digestate to struvite precipitation and ammonia stripping and absorption processes, but their 181 maximum gate prices were calculated as the product of their nitrogen and phosphorus content and the market values of the industrially synthesized (NH₄)₂SO₄³⁵ and (NH₄)₂HPO₄, ³⁶ expressed per kg of 182 183 nitrogen and phosphorus, respectively.

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The capital costs of the unit processes available in the current Cantabrian waste management plant (differentiated in Figure 1 with a discontinuous line) and the costs associated with the farmers' equipment and land were assumed to be already amortized. The capital costs of the other unit processes were annualized considering an amortization period of 15 years and a 7% interest rate, consistently with the Spanish banks' lending rates.³⁷

190 191 A previous study suggested that the GWI related to infrastructure do not constitute a significant fraction of the total GWI of waste management systems,³⁸ and therefore the GWI of the capital 192 193 goods were excluded from the analysis. 194 195 Another weakness of the model is that DNDC considers that all the phosphorus contained in the 196 organic fertilizers is in a mineral form that the crops can easily take up. Although this is a common supposition,³⁹ certain studies pinpoint that the products recovered from municipal organic waste 197 contain small amounts of organic phosphorus.⁴⁰⁻⁴² 198 199 200 201 Game theoretical model 202 203 The Stackelberg game is a sequential game model that makes a distinction between two types of 204 non-cooperative players - the leader and the followers - who do not coordinate their strategies and 205 only seek to optimize their own performance. The leader has the strategic advantage of making the initial decisions knowing how the followers will respond.⁴³ The Stackelberg game reflects the 206 207 hierarchical relationships between leaders and followers, and thus it was applied to model the case 208 study; the waste managers were identified as the leaders, who determine the quantities and prices 209 of the produced organic fertilizers, and the farmers, as the followers who decide which product to 210 purchase among the fertilizers available in the market. The waste managers must anticipate that, 211 given the choice between alternative fertilizing products that provide the same function, the 212 farmers will acquire the ones with the lowest associated costs. 213 214 215 **Optimization method** 216 217 The Stackelberg game was formulated as a bilevel optimization problem, in which the upper level 218 problem corresponds to the leader's problem, and the nested lower level problem, to the followers' problem.⁴⁴ To solve the bilevel problem, it was reformulated into a single-level problem by means 219 220 of the Karush-Kuhn-Tucker conditions, which – provided that the lower level problem is convex –

transform the lower level problem into a set of constraints appended to the upper level problem.⁴⁵

If the problem included discrete lower level variables, a more complex reformulation algorithm would be required.^{46,47} Reformulating the bilevel problem allows the upper and lower level problems to be solved concurrently to attain a Nash equilibrium where none of the players can improve their performance by unilaterally changing their actions; i.e., each player adopts the strategies that optimize their objectives given the actions taken by the other players.⁴³

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Although the minimization of the GWI of the entire system entails decisions in the upper and lower level problems, given the limited information that the followers have access to, and their more restricted decision-making power, the environmental objective function was considered as one of the leader's goals.⁴⁸ To simultaneously optimize the leader's environmental and economic objectives, a multi-objective optimization approach was adopted. Following the ε-constraint method,⁴⁹ a set of Pareto-efficient solutions – all of which are better than the others in at least one criterion – was obtained.

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237 **PROBLEM STATEMENT**

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The reformulated single level problem – a single period mixed integer linear program composed of 345,234 constraints, 148,470 continuous variables and 1,597 binary variables – was solved with the CPLEX algorithm⁵⁰ in an Intel^(R) Core^(TM) i7 CPU-4500U of 1.8 GHz and 8 GB of RAM. Setting the absolute optimality tolerance to 0, the computational time varied between 40 minutes and 27 hours, depending on the selected scenario and the defined constraints.

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246 Upper level problem

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The leader's profits were calculated as the sum of the annual revenues from the sale of organic fertilizers and the waste management tax paid by the municipalities minus the Total Annual Costs (TAC) of the waste management subsystem. To maximize the waste managers' profits and minimize the total GWI of the CIWMS, the leaders must make decisions on the configuration of the waste management subsystem and the price of the organic fertilizers.

254 The optimal design of the waste management subsystem is determined by the binary variables that 255 indicate which unit processes integrate this subsystem and the continuous variables that reflect the 256 amount of waste that each unit process handles. As Figure 1 illustrates, only the municipal organic 257 waste that has been source separated is allowed into the solid waste recycling processes (wet 258 thermophilic anaerobic digestion and tunnel or windrow composting); the organic waste that has 259 been mixed with inorganic materials must be sent to the landfill or the grate incinerator, along with 260 the solid rejects of the other unit processes. Hence, the Source Separation Rate (SSR) – the fraction 261 of municipal organic waste that is source separated – was identified as one of the leader's decision 262 variables.

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The price of the organic fertilizers was defined as an upper level decision variable that equates the sum of the product of a matrix of binary variables $(y_{p,r})$ and a matrix of parameters within the predefined range of gate prices $(FP_{p,r})$. This formulation allowed us to apply Glover's method⁵¹ to linearize the product of a continuous and a binary variable, ensuring that that the solutions to the optimization problem are global optimums.

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270 The system model relies on the assumption that all the produced organic fertilizers are sold to the regional farmers. This equation limits the amount of produced organic fertilizers (upper level 271 272 variable) to the total amount of organic fertilizers purchased by the farmers (lower level variable), 273 which is in turn restricted by the fertilization requirements of the regionally grown corn and wheat, 274 quantified in the lower level problem. Nevertheless, the mass balance that connects the waste 275 management and agricultural subsystems constitutes an upper level constraint because the waste 276 managers are the stakeholders in control of the production and sale operations. In addition to the 277 mass and energy balances that describe the waste management subsystem, the upper level problem 278 must satisfy these constraints:

• The waste managers' profits must be positive.

• Different types of composting processes cannot be concurrently integrated into the system.

Capacity restrictions. The minimal and maximal capacity restrictions of the waste management
 unit processes are shown in Table S47 of the Supporting Information. The minimal capacity
 restrictions were set as a requisite for the construction of new infrastructure to avoid the
 nonlinearities derived from the exponential equations that quantify how the TAC of the waste
 management unit processes decrease as the annual waste flows that they handle increase.⁵²⁻⁵⁷

These restrictions enabled us to assume that the incremental changes in the TAC with the incoming waste flows are constant. The validity of this assumption was investigated in Figures S10-S19, which compare the TAC considered in this study with the TAC exponential curves provided in the literature.^{55,57}

New waste management unit processes with the same function as those already present in the
 Cantabrian waste management plant can only be implemented if the capacities of the previous
 ones are exceeded.

In accordance with Directive 1999/31/EC,⁵⁸ the amount of landfilled biodegradable waste is
 limited to 35% of the total biodegradable municipal solid waste produced in 1995.

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297 Lower level problem

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The followers, who aim at maximizing their annual profits by reacting rationally to the leader's decisions, are the regional farmers that cultivate corn and wheat. Each farmer is characterized by their geographic location, the type of cereal they grow and the area they have available for crop production. A total of 63 followers were identified, only three of whom harvest wheat. Appendix E compiles the data that describe the farmers' activities, including the road distances from the agricultural sites to the waste management plant and to the two closest fertilizer plants, which are assumed to supply all the industrial fertilizers.

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The amount and type of fertilizers purchased by each farmer depend on the chosen fertilization strategy. To account for the fact that the nitrogen/phosphorus ratio in the organic fertilizers (excluding $(NH_4)_2SO_4$) is lower than the proportion of these nutrients required by corn and wheat, three fertilization strategies were defined:

Application of industrial fertilizers (NH₄NO₃ and (NH₄)₂HPO₄) to satisfy the crop demand for
 nitrogen and phosphorus. Farmers acquire these products from the nearest fertilizer plant to
 their fields.

Application of organic fertilizers to cover the crop nitrogen requirements. This strategy leads to
 excess phosphorus in the soil, unless (NH₄)₂SO₄ is applied, in which case (NH₄)₂HPO₄ must be
 added.

317 3. Application of organic fertilizers to supply the phosphorus needed by the crop. To correct the
318 nitrogen deficiency, NH₄NO₃ is provided.

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The followers' decisions are reflected by variable $xf_{c,m,p,s}$, which was defined as the amount of each type of fertilizer purchased by each farmer and applied to the soil in accordance with each fertilization strategy. The other variables and parameters involved in the lower level problem are described in the nomenclature section.

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325 The lower level problem was formulated as follows:

$$\max z(xf_{c,m,p,s}, y_{p,r}) \equiv \sum_{c \in C} \sum_{m \in M} \sum_{p \in P} \sum_{s \in S} \frac{CP_c \cdot Yield_{c,p,s}}{P_{c,p,s}} \cdot xf_{c,m,p,s}$$

$$-\left(\sum_{r \in R} FP_{p,r} \cdot y_{p,r} + IFP_{c,p} + sc + tc \cdot Dp_m\right) \cdot O_{c,m,p,s} \cdot xf_{c,mp,s}$$

$$-\left(\frac{\sum_{f \in F} CF_{c,f,p,s} \cdot \left(CFP_f + sc + tc \cdot Df_m\right) \cdot O_{c,m,p,s}}{P_{c,p,s}}\right) \cdot xf_{c,m,p,s} - (wc \cdot w_c + lc) \cdot At_{c,m}$$
(1)

s.t.
$$h_1(xf_{c,m,p,s}, Aorg_{c,m}) \equiv Aorg_{c,m} - \sum_{p \in P} \sum_{s \in S} \frac{xf_{c,m,p,s}}{P_{c,p,s}} \cdot Vorg_p = 0$$
 (2)

$$h_{2}(xf_{c,m,p,s}, Aorg_{c,m}) \equiv$$

$$\sum_{p \in P} \sum_{s \in S} xf_{c,m,p,s} \cdot Vfert_{s,p} - \left(\sum_{p \in P} \sum_{s \in S} P_{c,p,s} \cdot Vfert_{s,p}\right) \cdot (At_{c,m} - Aorg_{c,m}) = 0$$
(3)

$$g_{1}(xf_{c,m,p,s,r}, y_{p,r}, Aorg_{c,m}) \equiv$$

$$\sum_{p \in P} \sum_{s \in S} Vorg_{p} \cdot \left(\sum_{r \in R} FP_{p,r} \cdot G_{r,c,m,p,s} + sc \cdot xf_{c,m,p,s} + tc \cdot Dp_{m} \cdot xf_{c,m,p,s}\right)$$

$$+ Vorg_{p} \cdot \frac{\sum_{f \in F} CF_{c,f,p,s} \cdot (CFP_{f} + sc + tc \cdot Df_{m}) \cdot O_{c,m,p,s}}{P_{c,p,s}} \cdot xf_{c,m,p,s}$$

$$-Aorg_{c,m} \cdot \left(\sum_{p \in P} \sum_{s \in S} P_{c,p,s} \cdot Vind_{p} \cdot O_{c,m,p,s} \cdot (IFP_{c,p} + sc + tc \cdot Df_{m})\right) \leq 0 \quad \forall c, m$$

$$(4)$$

$$g_2(Aorg_{c,m}) \equiv Aorg_{c,m} - At_{c,m} \le 0 \quad \forall c,m$$
⁽⁵⁾

$$g_3(xf_{c,m,p,s}) \equiv xf_{c,m,p,s} - At_{c,m} \cdot P_{c,p,s} \le 0 \quad \forall c,m,p,s$$
(6)

$$g_4(xf_{c,m,p,s}) \equiv -xf_{c,m,p,s} \le 0 \quad \forall c,m,p,s$$
⁽⁷⁾

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The objective function was calculated as the annual revenues from the sale of grain minus the annual costs associated with fertilization (including the transportation and spreading of fertilizers), irrigation and labor.

Constraints h_1 and h_2 express that the total surface fertilized by the farmers must equal the area of their respective fields. Constraint g_1 captures the behavior of the followers in the Stackelberg game: if the cost of purchasing, transporting and spreading a given amount of organic fertilizers exceeds the cost of fertilizing the equivalent area with industrial fertilizers, the farmers will fertilize their fields solely with industrial fertilizers. Finally, constraints g_2 to g_4 indicate the upper and lower bounds of the lower level variables.

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339 - Reformulation of the lower level problem

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The leaders make their decisions prior to the followers, which allows the binary upper level variables that appear in the lower level problem $(y_{p,r})$ to be treated as parameters.^{43,45} In the absence of discrete variables, the lower level problem can be replaced by its Karush-Kuhn-Tucker conditions, which are composed of:

• Primal feasibility constraints. These are the lower level constraints: h_1 , h_2 , g_1 , g_2 , g_3 and g_4 .

Dual feasibility constraints. They are based on the derivatives of the lower level functions with
 respect to the lower level variables:

$$\frac{(CP_{c} \cdot Yield_{c,p,s} - \sum_{f \in F} CF_{c,f,p,s} \cdot (CFP_{f} + sc + tc \cdot Df_{m}) + vorg_{p} \cdot \mu 1_{c,m}) \cdot O_{c,m,p,s}}{P_{c,p,s}}$$

$$-\left(\sum_{r \in R} FP_{p,r} \cdot y_{p,r} + IFP_{c,p} + sc + tc \cdot Dp_{m} - vfert_{s,p} \cdot \mu 2_{c,m}\right) \cdot O_{c,m,p,s} - \left(\left(\sum_{r \in R} FP_{p,r} \cdot y_{p,r} + sc + tc \cdot Dp_{m}\right) + \frac{\sum_{f \in F} CF_{c,f,p,s} \cdot (CFP_{f} + sc + tc \cdot Df_{m})}{P_{c,p,s}}\right) \cdot O_{c,m,p,s} \cdot Vorg_{p} \cdot \lambda 1_{c,m} - \lambda 3_{c,m,p,s} \leq 0$$

$$\mu 1_{c,m} + \sum_{p \in P} \sum_{s \in S} P_{c,p,s} \cdot Vfert_{s,p} \cdot \mu 2_{c,m} - \sum_{p \in F} \sum_{s \in S} P_{c,p,s} \cdot Vind_{p} \cdot O_{c,m,p,s} \cdot (IFP_{c,p} + sc + tc \cdot Df_{m}) \cdot \lambda 1_{c,m} + \lambda 2_{c,m} = 0$$
(8)

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The domains of the auxiliary variables used to formulate the dual feasibility constraints are defined below:

351 $\mu 1_{c,m} \in \mathbb{R}$

| 352 | $\mu_{c,m} \in \mathbb{R}$ | |
|-----|--|------|
| | $\lambda 1_{c,m} \ge 0 \ \forall c,m$ | (10) |
| | $\lambda 2_{c,m} \ge 0 \ \forall c, m$ | (11) |
| | $\lambda 3_{c,m,p,s} \ge 0 \forall c,m,p,s$ | (12) |

Complementary slackness constraints. They indicate that the product of the left-hand side of
 the inequalities that compose the lower level problem and their associated dual variables must
 equal 0:

$$\lambda 1_{c,m} \cdot lhsg 1_{c,m} = 0 \tag{13}$$

$$\lambda 2_{c,m} \cdot lhsg2_{c,m} = 0 \tag{14}$$

$$\lambda 3_{c,m,p,s} \cdot lhsg3_{c,m,p,s} = 0 \tag{15}$$

$$lhsdf cx_{c,m,p,s} \cdot xf_{c,m,p,s} = 0 \tag{16}$$

358 Each complementary nonlinear slackness constraint was replaced by two equivalent linear 359 constraints using binary variables and a sufficiently large (or big-M) parameter:

$$\lambda 1_{c,m} \le y 1_{c,m} \cdot M_{c,m} \quad \forall \ c,m \tag{17}$$

$$-lhsg1_{c,m} \le (1 - y1_{c,m}) \cdot M_{c,m} \quad \forall c,m$$
⁽¹⁸⁾

$$\lambda 2_{c,m} \le y 2_{c,m} \cdot M_{c,m} \quad \forall \ c,m \tag{19}$$

$$-lhsg2_{c,m} \le \left(1 - y2_{c,m}\right) \cdot M_{c,m} \quad \forall c,m$$
⁽²⁰⁾

$$\lambda 3_{c,m,p,s} \le y 3_{c,m,p,s} \cdot M_{c,m,p,s} \quad \forall c,m,p,s$$
⁽²¹⁾

 $-lhsg3_{c,m,p,s} \le (1 - y3_{c,m,p,s}) \cdot M_{c,m,p,s} \quad \forall c, m, p, s$ (22)

$$xf_{c,m,p,s} \le y4_{c,m,p,s} \cdot M_{c,m,p,s} \quad \forall c, m, p, s$$
⁽²³⁾

$$-lhsdfcx_{c,m,p,s} \le \left(1 - y4_{c,m,p,s}\right) \cdot M_{c,m,p,s} \quad \forall c, m, p, s$$

$$\tag{24}$$

361 RESULTS AND DISCUSSION

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363 Before proceeding with the multi-objective optimization, the objective functions of the 364 reformulated single-level problem were separately optimized. The maximal profits that the waste 365 managers can earn, and the resulting GWI are represented in Figures 2A and 2C, whereas the profits 366 they would make if their only objective was to attain the minimal GWI (shown in Figure 2D) are 367 displayed in Figure 2B. In order to ascertain the influence of the uncertainty associated with the 368 behavior of the citizens responsible for waste generation and separation on the results, the single 369 objective optimization problems were solved for five SSR intervals (0≤SSR≤0.1, 0.1≤SSR≤0.2, 370 0.2≤SSR≤0.3, 0.3≤SSR≤0.4, 0.4≤SSR≤0.5); i.e., an optimal SSR was obtained for each interval.

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Figures 2A and 2B prove that, regardless of the SSR, the revenues derived from the sale of organic fertilizers are negligible with respect to the waste management tax. Moreover, the costs related to the collection and recycling of the source separated waste increase with the SSR, but the incineration and landfilling costs are reduced.

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The trade-off between the GWI of the waste management and agricultural subsystems is evidenced in Figures 2C and 2D. In general, as the SSR increases, the agricultural subsystem is responsible for more GWI because of the greater emissions associated with the transportation, spreading and soil application of the larger mass of organic fertilizers required to fulfill the fertilization needs compared with industrial fertilizers. Nonetheless, the GWI of the waste management subsystem decrease with the SSR because more waste can be processed by the anaerobic digestion and composting technologies instead of incinerated or landfilled

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Thus, as Figures 2A and 2D illustrate, the relationship between the SSRs and the optimal economic and environmental objectives could be described with a curve; the optimal profits and GWI are attained with the median SSR (0.25). However, that does not imply that the economic and environmental objectives follow the same trend. Figure 2B shows that the waste managers' profits would drop to nearly 0 if they only pursued a reduction in the GWI. These results provide grounds for the multi-objective optimization.



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392 Figure 2. Results of the single-objective optimizations of the leader's objective functions in the reformulated single-level problem for the defined

SSR intervals

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394 Figure 3A depicts the Pareto fronts and the prices of the organic fertilizers obtained for two 395 scenarios: i) the decentralized scenario described by the bilevel problem, and ii) a centralized 396 scenario wherein the farmers' economic interests are disregarded. The latter was optimized solving 397 the upper level problem subject to the restrictions of the lower level problem. Both Pareto fronts 398 confirm that the optimal SSR range is 0.2-0.3, and that the improvement in the GWI is accomplished 399 at the expense of the waste managers' profits. The amount of digestate produced is progressively 400 reduced as the restriction on the GWI is relaxed, allowing the waste managers to increase their 401 profits.

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403 The balance between the farmers' and waste managers' economic interests in the decentralized 404 scenario is reflected in the lower prices set for the organic fertilizers (0-2 € metric ton⁻¹ of compost, 405 and 0-1 € metric ton⁻¹ of digestate), whereas in the centralized scenario the waste managers set the 406 maximum prices allowed by the restrictions of the lower level problem. The results of the 407 decentralized scenario are more consistent with the symbolic prices that European farmers usually pay for organic fertilizers.³²⁻³⁴ The digestate is assigned lower prices than compost to compensate 408 409 for the larger mass of digestate required to achieve the same fertilizing function, and therefore the 410 digestate transportation and spreading costs are higher than those of compost.

411

412 The farmers' better economic performance in the decentralized scenario is accompanied by a 413 reduction in the waste managers' profits and increased GWI with respect to the centralized scenario. 414 This happens because the solutions to the bilevel problem rely to a greater extent on the use of the 415 organic fertilizers to cover the crops' phosphorus requirements, which reduces the amount of 416 $(NH_4)_2$ HPO₄ needed. This fertilization strategy is based on the application of NH₄NO₃, a fertilizer that 417 is less expensive than (NH₄)₂HPO₄, but also has a higher carbon footprint. Nevertheless, as Figure 3A 418 shows, the relative differences between the leader's economic and environmental objectives in 419 both scenarios are not remarkable. This can be attributed to the small fraction of the revenues due 420 to the sale of organic fertilizers, and to the low contribution of the agricultural subsystem to the 421 overall GWI.









Figures 2 and 3A show that the waste managers' margin for profits and environmental improvement are quite slight. However, the decision-makers can push the Pareto frontier changing some of the fixed operating decisions that act as model parameters. Since the waste management tax is the main source of income to the waste managers and hence it will determine the feasibility of the CIWMS, a sensitivity analysis considering increases of 25% and 50% in the current waste management tax was carried out for the decentralized scenario. The resulting Pareto fronts are presented in Figure 3B.

432 Raising the waste management tax could bring about reductions of up to 19% in the GWI, which are 433 significant compared with the maximal 11% reduction that can be achieved with the current tax. 434 The reason is that the minimal GWI are no longer limited by the restriction on the minimal profits 435 that the waste managers must make. The rise in the revenues allows the waste managers to 436 implement larger SSRs; the scenarios with the increased waste management taxes attain the 437 minimal GWI based on a 49% SSR, the valorization of all the source separated organic waste in the 438 anaerobic digester, and the ammonia stripping and absorption of the liquid digestate, which enables the sale of (NH₄)₂SO₄ for prices between 29 and 43 € metric ton⁻¹. However, the optimal SSR the 439 440 waste managers should implement to maximize their profits irrespective of the tax is 25%.

441

442 The results of Figure 4 – which indicates the geographic location of the regional farmers and the 443 type of organic fertilizers they purchase –correspond to the Pareto optimal solutions that generate 444 $54x10^{6}$ kg CO₂-eq·year⁻¹ in the decentralized scenario. For all the analyzed waste management taxes, 445 the farmers that purchase the organic fertilizers are located within a 32 km radius around the waste 446 management plant; the farmers located further away opt to purchase industrial fertilizers to reduce 447 the transportation costs. In the scenario with the highest waste management tax, struvite is 448 produced at a price of 58.49 € metric ton⁻¹. Struvite is the fertilizer sent to the farthest agricultural 449 site because of the lower amount of product required to fertilize the same area relative to the other 450 organic fertilizers.

451

The individualized recommendations that can be made to the farmers and the waste managers based on these results prove that the integration of life cycle and game theoretical models constitutes an improvement with respect to the existing centralized life cycle optimization frameworks.



475 colored circles is proportional to the area fertilized with the organic fertilizers

476 **CONCLUSIONS**

477

The proposed optimization framework allows the analysis of the environmental and economic consequences of the adoption of a circular economy through the lens of all the stakeholders, and the simultaneous optimization of their decisions in accordance with their conflicting objectives.

481

The results demonstrate that a deviation from the objective of economic growth – understood as an increase in profits – is needed to achieve a reduction in the GWI. To improve the competitiveness of the organic fertilizers in the market, their prices must be set quite low with respect to the industrially produced fertilizers. Therefore, the sale of organic fertilizers constitutes an insignificant source of revenues for the waste managers; without economic incentives that spur the investment in novel technologies, it is unlikely that waste managers will change their mindset and start viewing organic wastes as valuable products.

489

Moreover, an 11% reduction in the GWI of the system can be achieved at most with the current
waste management tax, which suggests that the implementation of a circular economy is not the
most effective strategy to combat climate change.

493

Although these results cannot be extrapolated to other case studies, the developed framework can be adapted to different systems. Future studies should model the behavior of the agents that generate waste, who determine the amount of waste that is source separated and will be affected by the changes in the waste management tax and the cost of staples.

498

The further improvements and deployment of this framework could bridge the gap between the theoretical concept of a circular economy and its industrial applications, helping policy-makers devise a roadmap to attain a sustainable circular economy.

| 502 | ABBREVIAT | IONS |
|------------|---|---|
| 503 | CIWMS | Circular Integrated Waste Management System |
| | GWI | Global Warming Impacts |
| | LCA | Life Cycle Assessment |
| | SSR | Source Separation Rate |
| | TAC | Total Annual Costs |
| 504 | | |
| 505 | | |
| 506 | NOMENCLA | ITURE |
| 507 | | |
| 508 | Sets | |
| 509 | C crops | |
| 510 | F Industrial | fertilizers |
| 511 | <i>M</i> Municipa | lities |
| 512 | P Fertilizers | |
| 513 | R Prices of t | he organic fertilizers |
| 514 | S Fertilizatio | on strategies |
| 515 | | |
| 516 | Upper level | variable |
| 517 | <i>y_{p,r}</i> Binary d | ecision on the price of the organic fertilizers |
| 518 | | |
| 519 | Lower level | variables |
| 520 | Aorg _{c,m,p,s} Ar | rea fertilized with the organic fertilizers (ha) |
| 521 | <i>TFC_{c,m,p,s}</i> Tot | al costs related to the purchase, transportation and spreading of the fertilizers (${f \in} \cdot$ ha ⁻¹) |
| 522 523 | <i>xf_{c,m,p,s}</i> Amo accordance | unt of each fertilizing product purchased by each follower and applied to the soil in with each fertilization strategy (kg) |
| 524 | | |
| 525 | Reformulat | ion variables |
| 526 | μ1 _{c,m} , μ2 _{c,m} , λ1 | $L_{c,m}$, $\lambda_{2_{c,m}}$, $\lambda_{3_{c,m,p,s}}$ Continuous variable used to define the dual feasibility constraints |

- $G_{r,c,m,p,s}$ Auxiliary variable used to apply Glover's linearization method and equal to the product of 528 $xf_{c,m,p,s}$ and $y_{p,r}$
- *Ihsdfcx*_{c,m,p,s} Left-hand side of the dual feasibility constraint based on the derivatives with respect to 530 $xf_{c,m,p,s}$
- *Ihsg1_{c,m}, Ihsg2_{c,m}, Ihsg3_{c,m,p,s}* Left-hand side of constraints g1-g3
- $Y_{1_{c,m}}, Y_{2_{c,m}}, Y_{3_{c,m,p,s}}, Y_{4_{c,m,p,s}}$ Binary variables used for the linearization of the complementary 533 slackness constraints

535 Parameters

- 536 At_{c,m} Total fertilized area (ha)
- $CF_{c,f,p,s}$ Amount of industrial fertilizers required to complement the fertilization of 1 ha with organic 538 fertilizers (kg·ha⁻¹)
- *CFP_f* Gate price of industrial fertilizers ($\epsilon \cdot kg^{-1}$)
- CP_c Crop price ($\mathbf{\in}$ -metric ton⁻¹)
- Df_m Distance from the industrial fertilizer plant to the fields (km)
- $Dp_{m,p}$ Distance from the fertilizer production sites to the fields (km)
- $FP_{p,r}$ Gate price of fertilizers ($\mathbf{\in kg^{-1}}$)
- *IFP_{c,p}* Average gate price of the industrial fertilizers required to fertilize each crop (ϵ kg⁻¹)
- *lc* Labor costs (€·ha⁻¹)
- *M_{c,m}* Matrix of large parameters
- *M_{c,m,p}, M_{c,m,p,s}* Tensors of large parameters
- *O_{c,m,p,s}* Tensor of zeros and ones indicating the possible combinations of c, m, p and s
- $P_{c,p,s}$ Amount of fertilizers required to fertilize 1 ha (kg·ha⁻¹)
- 550 sc Spreading costs (€·kg⁻¹)
- *tc* Transportation costs (€·kg⁻¹·km⁻¹)
- 552 TCFC_{c,m,p,s} Total costs related to the purchase, transportation and spreading of the industrial
- fertilizers required to complement the fertilization of 1 ha with organic fertilizers (ϵ -ha⁻¹)
- *Vfert*_{p,s} Matrix of ones and zeros indicating the selection of industrial fertilizers</sub>
- *Vind_p* Vector of ones and zeros indicating the selection of the industrial fertilizers

- *Vorg_p* Vector of ones and zeros indicating the selection of the organic fertilizers
- w_c Water requirements (m³·ha⁻¹)
- 558 wc Water costs (€·m⁻³)
- *Yield*_{c,p,s} Crop yield (metric ton \cdot ha⁻¹)

562 SUPPORTING INFORMATION

563 Model parameters, DNDC, LCA and Life Cycle Costing results.

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- 799 A multi-objective optimization framework integrating life cycle and Stackelberg models was
- 800 developed to design sustainable circular waste management systems