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Unlocking advanced waste management models: Machine learning integration of emerging technologies into regional systems

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ABSTRACT

The waste management sector requires specialized systems analysis tools to facilitate decision-making and make waste management sustainable and efficient. While integrated systemic approaches exist for assessing conventional waste management systems, the integration of emerging technologies such as gasification, pyrolysis, and methane dry reforming remains largely overlooked. In this work, these three technologies have been integrated into a conventional regional waste management model by abstracting rigorous simulation models into machine-learning surrogate models. The resulting technology-rich waste management model incorporates material flow analysis and life-cycle assessment as tools for supporting policy and decision-making. The model was tested by assessing the environmental impacts and landfill rates for three technology implementation scenarios. Overall, the inclusion of these emerging technologies led to an environmental performance improvement compared to a reference system. For example, a 116.5 % reduction of the carbon footprint in the most optimistic scenario. Nevertheless, the mere addition of these technologies was not enough to achieve landfill rates below 10 %, reaching 37.6 % in the most optimistic scenario. Therefore, properly sizing capacity was found to be a key factor in minimizing both environmental impact and landfill rate.

1. Introduction

Over 2.2 billion tons of waste are generated every year in the European Union. Municipalities have to deal with 27 % of the total waste, mainly generated by households, but also commercial activity and street waste collection (EU Monitor, 2023). Economic growth coupled with an increasing population that is expected to live mainly in urban areas (70 % globally by 2050) emphasizes the need to find sustainable solutions to the associated waste generation (Abubakar et al., 2022; Hoornweg and Bhada-Tata, 2012). Inadequate waste management, ranging from absent collection systems to inefficient disposal methods, leads to a loss of valuable resources as well as greenhouse gas (GHG) emissions, air pollution, water contamination, and soil degradation, amongst other impacts (UN Environment Programme, 2017).

Over the years, the waste management sector has transitioned from regulation-driven end-of-pipe solutions like landfilling to high-value operations involving materials and energy recovery (Aid et al., 2017). The European Commission's Directive 2018/850 on the landfill of waste aims to prevent or reduce adverse environmental effects from waste landfilling and sets a target for municipalities for 2035, when the landfill rate should not exceed 10 % (European Commission, 2018; European Environment Agency, 2024). European countries that already have a landfill rate well below the limit such as Germany, Austria, Denmark and Belgium rely heavily on recycling to do so, while others accomplish it by using incinerators such as Norway, Sweden and Finland (European Environment Agency, 2023, 2024). Even though incineration is recognized as a way to prevent waste from reaching landfills while generating electricity and/or heat (Istrate et al., 2021a), it was excluded from European funding instruments such as the Recovery and Resilience Facility in 2021 (European Commission, 2021). This instrument declared that the construction of new incinerators was an example of non-compliance with the Do No Significant Harm (DNSH) principle (European Commission, 2023) as they are carbon-intensive processes that undermine the efforts to decrease GHG emissions and harm business models that could improve circularity (Oliveira, 2021). However, phasing out incineration without any alternative treatment leads to a direct increase in the landfill rate and the subsequent environmental impacts, even if source separation of waste is increased (Istrate et al., 2021a).

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As waste management systems (WMSs) have progressed with the introduction of advanced technologies and the establishment of various markets for recovered products (i.e., materials, energy, and nutrients), waste management planning has turned increasingly complex (Eriksson and Bisaillon, 2011). Notably, the development of emerging technologies such as gasification, pyrolysis, and dry reforming of methane creates opportunities for obtaining high-value products from waste, including methanol, hydrogen, and synthetic diesel and gasoline (Abdelsadek et al., 2023; Cheng et al., 2023; Ouedraogo et al., 2021). Consequently, managers face uncertainty as these emerging waste valorization technologies come into play, especially to replace incinerators. On the one side, their implementation might become imperative to meet regulation. On the other side, very little information on their integration into WMSs is available to make informed decisions regarding their technical or environmental impacts.

Systems analysis tools for WMSs can help close the gap between waste managers, technology developers, researchers and policy-makers by supporting the decision-making process and providing realistic performance expectations. Systemic approaches based on material flow analysis (MFA) have proven useful in providing a comprehensive model of the flow of materials and substances through a WMS (Di Nola et al., 2018; Istrate et al., 2021a, 2021c). The aforementioned model has to consider the interactions between the physico-chemical composition of the managed waste, the performance of the technologies used to deal with it, and the required inputs (energy, raw materials, natural resources, etc.) and outputs (emissions, products, etc.). Thus, the MFA-based model needs to be improved upon by incorporating life-cycle assessment (LCA). In this regard, LCA has gained traction in supporting policy and decision-making as it evaluates the potential environmental impacts of the system as a whole (Hunsager et al., 2014; Liu et al., 2016; Margallo et al., 2019; Pryshlakivsky and Searcy, 2021; Thushari et al., 2020).

Nevertheless, while individual studies covering the environmental impacts of emerging technologies like gasification, pyrolysis and dry reforming can be found in the literature (Azam et al., 2022; Ouedraogo et al., 2021; Zaman, 2013; Zhu et al., 2022), none of them offers a system perspective on their integration into a complete WMS. This knowledge gap poses a challenge as waste managers seek to improve the performance of the entire system rather than just individual technologies or waste streams. Therefore, it is crucial to uncover the potential system-wide benefits of integrating emerging technologies to attract investment attention (Thyberg and Tonjes, 2015). The lack of a systemic approach in the literature is largely attributed to the complexity of developing reliable models that can seamlessly integrate into MFA-based WMS superstructures. Traditional MFA approaches rely on static transfer coefficients for input materials, whereas this study introduces an innovative approach by employing machine learning-based surrogate models. These models correlate the variability in technical and environmental performance of emerging technologies with operational parameters and waste input characteristics, addressing limitations in conventional modeling approaches.

Previous modeling efforts have focused on rigorous simulations at the individual technology level (Azam et al., 2022; Mehdi et al., 2023), whose complexity prevents their integration into a generic MFA and LCA model of a WMS. In this sense, surrogate or substitute models were found to be used in literature for abstracting these complex simulations into black box machine-learning surrogate models (Cheng et al., 2023; Ishitsuka and Lin, 2023). This abstraction involves deriving meaning from descriptive datasets. The advantage of using machine-learning substitute models is that they are computationally light to run and capable of retaining the responsiveness of a rigorous simulation. However, to the best of the authors' knowledge, black box surrogate models for emerging waste treatment technologies and their subsequent integration into a system-level WMS model have not been explored so far. Yet, it constitutes an innovative methodological approach for estimating the technical and environmental performance of emerging technologies while helping waste managers make sustainability-oriented decisions.

Within this context, the present work aims to fill the gap of a systemic approach by developing an integrated MFA and LCA model for a WMS capable of quantitatively evaluating the integration of emerging waste treatment technologies. To achieve this, the following specific objectives had to be accomplished:

– To prepare individual simulation models for waste gasification, waste pyrolysis, and biogas dry reforming.
– To prepare machine-learning surrogate models and integrate them into an MFA and LCA model of a WMS.
– To evaluate a set of three technology integration scenarios from a technical and environmental perspective to illustrate the decision-making value of the generated model.

2. Methodology

2.1. Conceptualization

In order to fill the above-mentioned gap, this work builds on top of the waste management model developed by Istrate et al. (2021b). This is an integrated MFA and LCA model for tracking the flow of substances and materials throughout the WMS and quantifying the associated environmental impacts. The core structure is formed by all blocks and streams colored in black in Fig. 1. The key aspect of this model is its capability to predict the performance of waste management processes according to changes in the composition and characteristics of the input waste stream. This is achieved by mathematically linking process inputs and outputs to the mass and biological and chemical properties of the treated waste stream through transfer coefficients or simplified process models (e.g., CO_2 emissions from incineration are linked to the carbon content of the input waste).

In addition to process mass and energy balances, the model implements capacity constraints, limiting the amount of waste that could be treated by each process within the WMS. Specific details on the configuration and modeling of conventional waste management processes can be found in Istrate et al. (2021b). In terms of waste generation, the model deals with the following materials: food waste, green waste, mixed paper, cardboard, polyethylene terephthalate (PET), high-density polyethylene (HDPE), low-density polyethylene (LDPE), mixed plastic, cartons and alike, glass, ferrous metal, non-ferrous metal, textile, wood, and other. They are all characterized in detail in terms of ultimate composition and other physico-chemical properties such as lower heating value.

The conventional WMS modeled by Istrate et al. (2021b) was found to rely heavily on incineration to avoid landfilling. To achieve a low landfill rate, additional measures such as the implementation of new waste management processes need to be implemented, in particular waste gasification and pyrolysis. Even though these technologies are well known to the scientific community, they are only now starting to be considered by waste managers for field-scale operations. Other technologies such as dry reforming are also in the development phase to generate syngas from the biogas produced in the anaerobic digester. Fig. 1 presents a modified version of the conventional WMS, in which the three mentioned technologies have been introduced in the system. Gasification (green in the upper part of the figure) and pyrolysis (yellow) aim to help in phasing out incineration and produce syngas (in the case of gasification) and pyr-oil and char (in the case of pyrolysis), while dry reforming of methane (green in the bottom part of the figure) arises as a biogas utilization pathway to produce also syngas.

Fig. 2 presents the methodological framework to model and assess the mass and energy flows within the WMS. Two different levels can be distinguished: process level and system level. The process level involves process simulation itself, the generation of machine-learning substitute models, and the life-cycle inventory (LCI) models for each process. The system level refers to the integration of these models into the WMS and

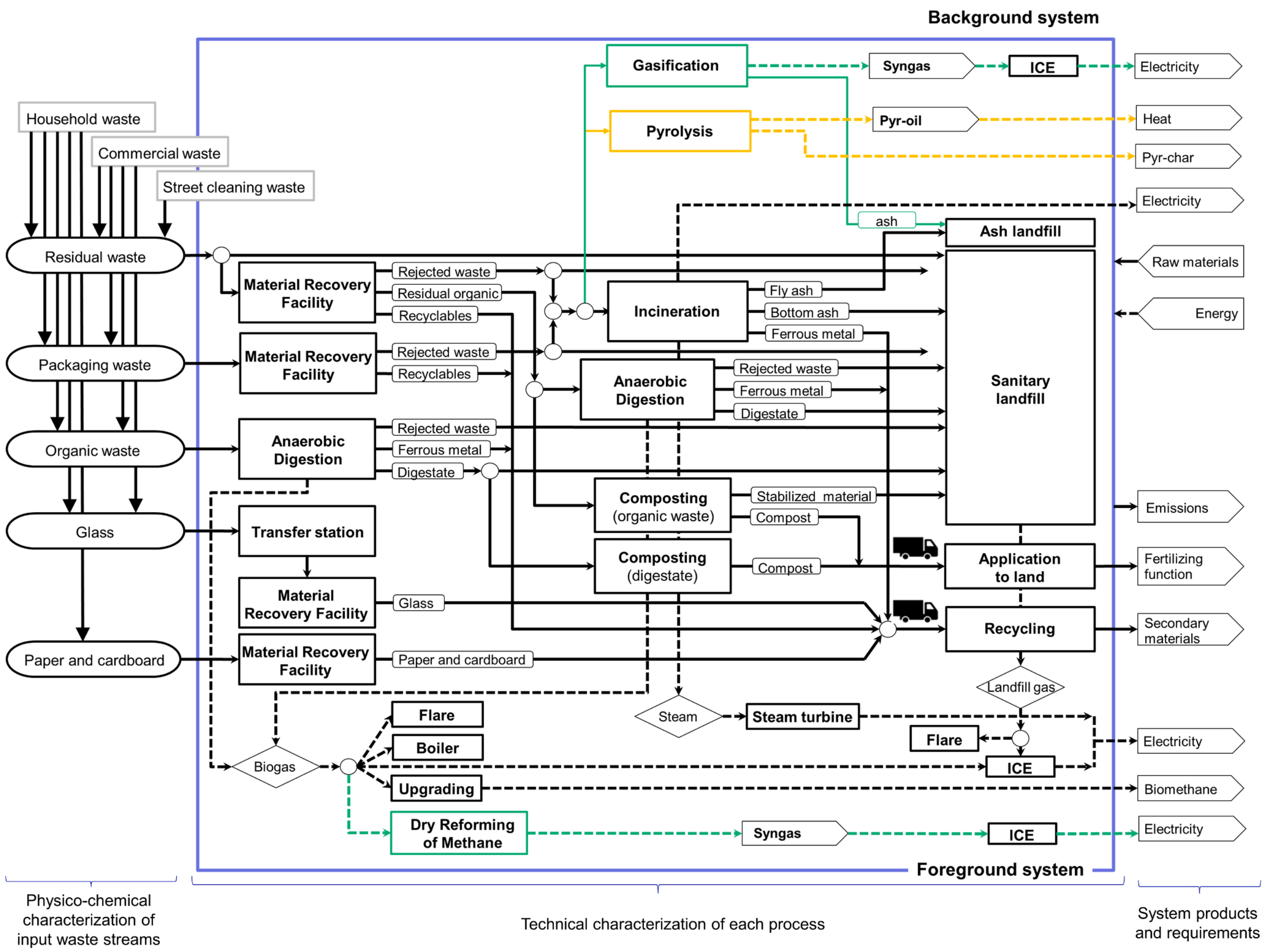

Fig. 1. Updated WMS structure considering the integration of emerging treatment technologies. Solid lines represent mass flows, whereas dashed lines represent energy-relevant flows. ICE: internal combustion engine. Adapted from Istrate et al. (2021b).

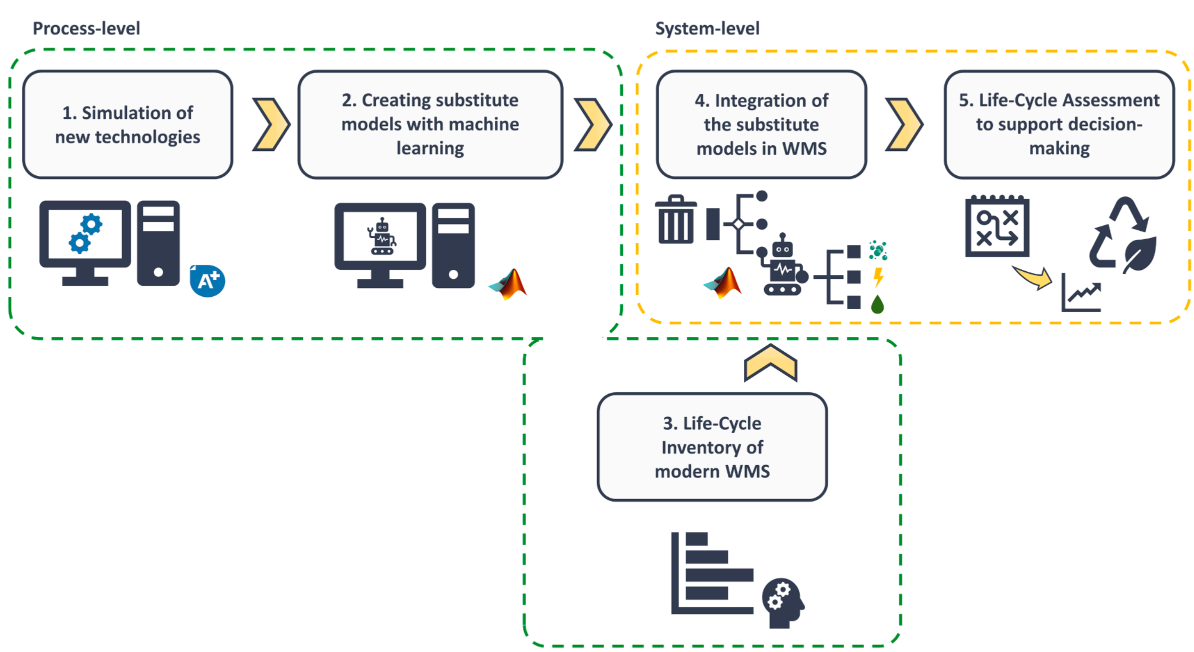

Fig. 2. Methodological approach followed in this work for the assessment of a regional waste management system (WMS).

the LCA-based decision-making that follows.

At the process level, mass and energy balances of conventional blocks such as material recovery facilities (MRFs), anaerobic digestion or incineration were modeled in Istrate et al. (2021b) primarily through transfer coefficients. In contrast, in the case of the new technologies, transfer coefficients are not readily available due to the lack of industrial-scale facilities. Therefore, these technologies were implemented as black-box models coming from the abstraction of Aspen Plus (AspenTech, 2025) simulations using machine learning. To do so, the first step was to prepare and consolidate individual simulation models in Aspen Plus for each of the new technologies (Section 2.2).

Afterward, synthetic data was generated through sensitivity analysis and used to train the corresponding machine-learning surrogate model. This innovative approach incorporates the embedded thermodynamic responsiveness from the rigorous simulation into the MFA model, which is especially important as gasification and pyrolysis are very dependent on operating conditions and composition of the feedstock (Shah et al., 2023). Once these simpler models were integrated into a new iteration of the WMS model (Section 2.3), this new configuration of the WMS was used to produce LCI data for the complete system (Section 2.4), enabling the system-level analysis of different scenarios (Section 2.5). The required ecoinvent v3.10 cut-off datasets were used for local calculations within the model to perform the LCA and obtain the corresponding life-cycle profiles.

2.2. Modeling of new technologies

This section delves into the specifics of the process simulation required for the first methodological step.

2.2.1. Gasification

The gasification process consists of four internal steps, drying, pyrolysis, combustion (oxidation), and gasification (reduction), which occur differently depending on process configuration, as shown in Fig. 3a. This process leads to the formation of simple molecules, primarily syngas (mainly composed of hydrogen and carbon monoxide), which can be further utilized for electricity generation or converted into synthetic fuels or hydrogen (Tan et al., 2024).

In the gasifier, drying happens within the temperature range of 100 °C to 150 °C, pyrolysis takes place between 200 °C and 700 °C, combustion occurs within the range of 700 °C to 1500 °C, and gasification happens between 800 °C and 1100 °C. Typically, municipal waste contains moisture levels ranging from 5 % to 35 %, reaching values below 5 % during the drying process. During pyrolysis, municipal waste undergoes heating in the absence of oxygen, causing its volatile components to vaporize. These volatile vapors constitute a mixture of hydrogen, carbon monoxide, carbon dioxide, methane, hydrocarbon gases, tar, and water vapor (Kivisaari et al., 2004; Shah et al., 2023). In the combustion step, oxygen supplied to the gasifier interacts with the combustible substances, leading to the formation of carbon dioxide (CO_2) and water (H_2O). These compounds then undergo reduction upon contact with the char produced from pyrolysis (Safarian et al., 2019a; Shah et al., 2023). Reduction processes yield syngas, a mix of combustible gases such as hydrogen, carbon monoxide, and methane (Safarian et al., 2019b). Regarding configurations for the gasification process, downdraft, updraft, fluidized bed, and circulating fluidized bed gasifier simulation models were prepared (Shah et al., 2023). The studied configurations were reflected in an Aspen Plus specific gasification hierarchy block, detailed in the Supplementary Information, and then integrated into the gasification general simulation shown in Fig. 3a.

All four gasification models followed the same general structure. First, an input selector was configured through an Excel subroutine using a calculator, enabling the option to simulate variating feedstocks using their ultimate composition. In this way, combinations of different types of waste can be calculated and fed to the model as long as their ultimate composition is known. The external drying step follows the input selector, reducing moisture to at least 12 %. In the next step, the feed is taken to the gasification process itself. In this case, the gasification block is different for every simulation depending on the studied configuration. Each specific configuration is implemented in the block A200. The simulation of each configuration can be found in the Supplementary Information. They all consist of a drying step followed by an RYield block, the Aspen Plus yield reactor, which was used to simulate feedstock decomposition. In this section, the feedstock is transformed from a non-conventional solid to volatile materials (VMs) and char. The VMs include hydrocarbons, oxygen, hydrogen, carbon monoxide, and non-combustible gases, while char is transformed into ash and carbon. VM yield is equal to the volatile content in the waste feedstock determined by the proximate analysis (Safarian et al., 2022). After the decomposition step, the VMs are sent to the oxidation and reduction steps modeled with an RGibbs block. The order depends on the specific configuration and each of them can be explored in detail in the Supplementary Information. In all cases, industrially relevant parameters such as steam-to-biomass ratio or the equivalence ratio can be individually configured.

2.2.2. Pyrolysis

In comparison to incineration, pyrolysis decomposes waste at lower temperatures, typically ranging between 350 and 900 °C, within an oxygen-deficient environment or, in specific instances, with very low oxygen concentrations to enhance the heating rate and yield a greater amount of gas. The resulting pyrolysis oil product can be refined into diesel and other petrochemical materials.

Modeling the pyrolysis of waste is a challenging task. Equilibrium models have trouble predicting the product composition, especially in the liquid phase, where they tend to overestimate the presence of water. On the other hand, other types of models such as kinetic ones produce valid results for a limited number of feedstocks and reactors. For these reasons, a novel approach was selected in the modeling of this process, based on the combination of an artificial neural network with Aspen Plus (Martínez-Ramón et al., 2024a). For pyrolysis, the proportion of gas, oil, and char is strongly dependent on the reaction temperature, residence time, and, especially, waste composition. The artificial neural network was trained in MATLAB to predict the yield for the gas, liquid, and solid phases and their approximate composition based on the experimental results from different plastic pyrolysis experiments gathered from literature by Cheng et al. (2023). The resulting MATLAB function was then called from an Excel calculator in Aspen Plus and run under the operating conditions of the simulation. The yields for representative components of the three resulting phases estimated by the neural network were exported onto the RYield reaction block (NN-PYR in Fig. 3b) representative of the pyrolysis reactor. Following the reactor, the solid char was separated from the gases with a cyclone and the resulting gas mix cooled to 50°C, obtaining the main product (pyrolysis oil) together with a mix of pyrolysis gases that were subsequently burned to supply the required heat to the pyrolysis reactor (Fig. 3b).

2.2.3. Dry reforming of methane

Dry reforming of methane (DRM) is widely studied as one of the potential routes for syngas production from biogas. In this work, a chemical looping configuration of this process was considered, which is expected to increase the yield of syngas and optimize CO_2 activation, additionally avoiding side reactions and the need for complex catalyst regeneration systems. The DRM unit consists of a fixed bed reactor that operates in two different modes: reaction and regeneration. In the reaction step, the biogas is fed to the fixed bed reactor operating at 900 °C to generate syngas, used to preheat the biogas feed. The system contemplates using three different catalysts (cerium, ferrite, and zinc oxide), which are regenerated through calcination. This system was implemented in Aspen Plus according to Martínez-Ramón et al. (2023, 2024b). The sensitivity analysis results obtained from the simulation are illustrated in the process-level results section of this work (Section 3.1).

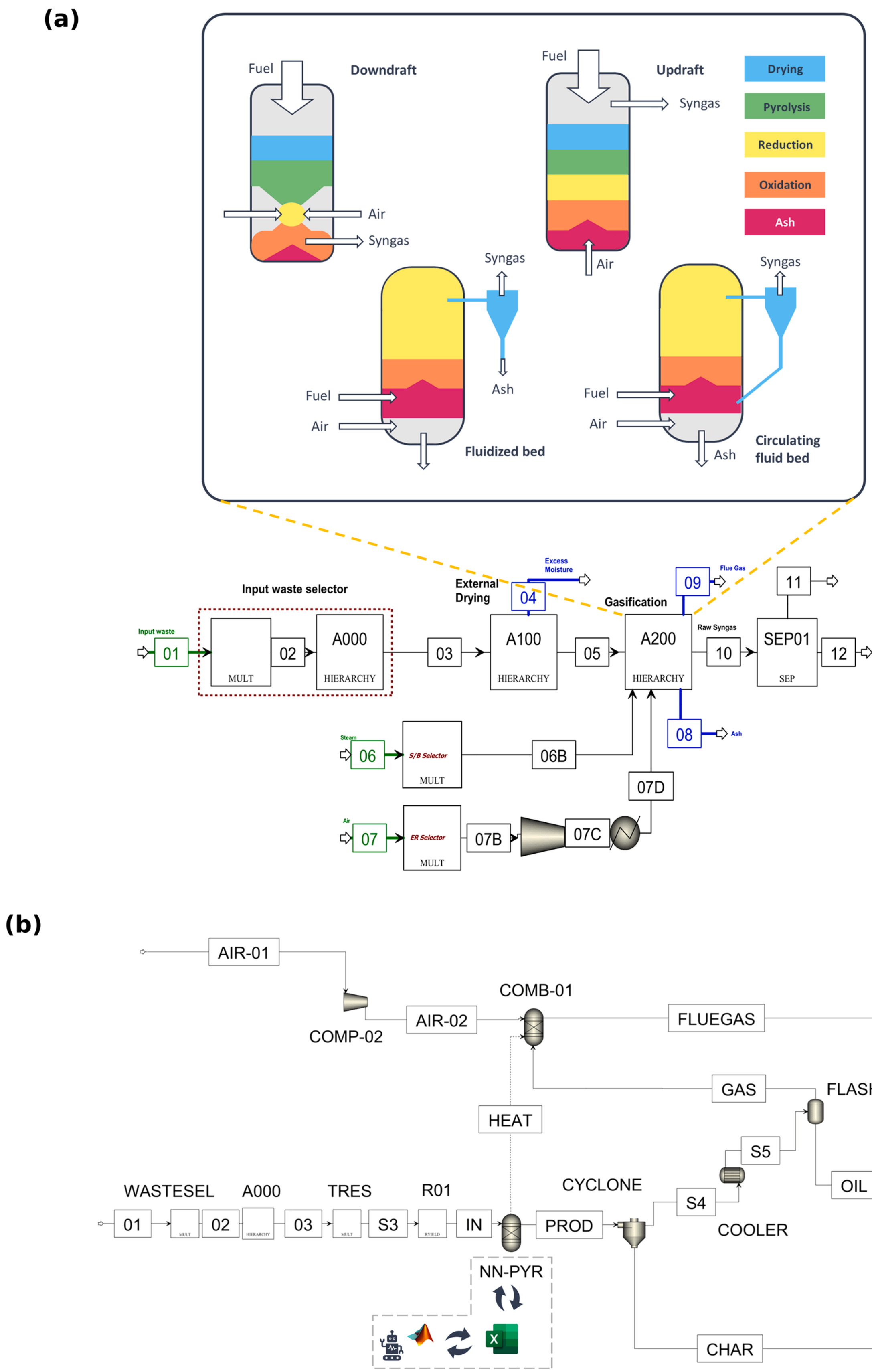

Fig. 3. (a) General gasification simulation, where each specific configuration is implemented in the block A200, and (b) Aspen Plus simulation diagram for waste pyrolysis.

2.3. Generation and integration of machine-learning surrogate models

Connecting an Aspen Plus simulation model to the WMS model built in MATLAB can be complicated. Furthermore, executing all three simulations every time the WMS model is run is a computationally demanding task. To address this, machine-learning surrogate models were trained to substitute the Aspen Plus rigorous models. For this strategy to be valid, the surrogate models have to retain the physical meaning of the Aspen Plus simulations. To that end, the Aspen Plus models were used to produce synthetic data through process-level sensitivity analysis by examining how changes in model parameters or variables affect process performance or output variables. Consequently, descriptive variables for each of the three technologies had to be selected and varied within specific ranges. The composition of the feedstock, either waste or biogas, and the temperature and the pressure in the reactors were the main variables. Additionally, each process has some intrinsic characteristics (e.g., the used catalyst for the dry reforming or the type of gasifier used in the gasification simulations) which were saved as categoric variables in the datasets. Table 1 presents the range of operating conditions for each descriptive variable, the number of points used to describe that range, and the tracked responses (results from the simulation) which will be the outputs from the machine-learning surrogate models.

Once obtained, each of the three datasets (available as Supplementary Information) was used to train a machine-learning regression model. Simulation runs that returned an error during the sensitivity analysis were removed from the dataset. Artificial neural networks were selected as machine-learning algorithms given their capacity for handling complex and nonlinear relationships in multivariate systems (Montesinos López et al., 2022). A key step in the formulation of a valid machine-learning model is the training process, taking special care to avoid overfitting (Manashgoswami, 2023). In order to ensure a model with high generalization capacity, all datasets were first randomized. Additionally, Bayesian regularization was selected as the training algorithm as it improves generalization (MathWorks, 2025). However, for this type of algorithm to work best, network inputs and targets should fall in the range of −1 to 1. Subsequently, these values were normalized to have zero as the mean and unity as the standard deviation (MathWorks, 2023). Different architectures were used for each of the surrogate neural networks. The neural network used in the case of the gasification process used 2 layers of 42 and 21 neurons each. In the case of DRM, one layer with 20 neurons was used; in the pyrolysis surrogate, two layers of 25 and 13 neurons each were used.

The generated models were deployed in the WMS model. To do so, they were called as MATLAB functions and fed all the necessary information to be run (column "Input" in Table 1). The operational parameters such as configuration, temperature, pressure, or vapor residence time were set up manually for each scenario, however the ultimate composition of the feedstock was read from the feed stream going into the process. Once run, the models return the outputs (column "Output" in Table 1) that compile the necessary variables to estimate the LCI for these newly integrated processes. In parallel, major inventory variables for the rest of the processes in the model are calculated according to the technical characterization established in Istrate et al. (2021b). These variables are depicted in Fig. 1 as "System products and requirements".

2.4. Life-cycle assessment

LCA is spread across both process and system level. At the process level, LCIs were calculated for every process in the WMS. At the system level, the use of these LCIs together with the ecoinvent database (Wernet et al., 2016) enabled the assessment of the potential environmental impacts of the complete WMS. The functional unit of the study was defined as the yearly amount of waste generated in the city of Madrid as it is a large city with an established waste management system that discloses activity reports yearly. Waste was considered as the sum of household, commercial, and street cleaning waste and it adds up to 1394,105 tons per year according to local activity reports (Municipality of Madrid, 2025).

Table 1
Parametric description of the sensitivity analysis.

Input	Units	Range	Number of points	Output
Dry reforming of methane				
Temperature	°C	650 - 1000	12	CO_2 in syngas [kmol/year], CH_4 in syngas [kmol/year], H_2 in syngas [kmol/year], CO in syngas [kmol/year], water in syngas [kmol/year], heat requirement [kW], electricity requirement [kW], cooling water [kg/h]
Pressure	bar	0.1 - 0.99 and 1 - 8	12×2	
Methane composition in biogas	%	35 - 75	12	
Catalyst used	-	Cerium, ferrite and zinc oxide	3	
Gasification				
Type of gasifier	–	Circulating, downdraft, fluidized, and updraft	4	Syngas production [kg/h], syngas composition (water, H_2, CO, CO_2, CH_4), higher heating values for dry and wet syngas [MJ/kg], higher heating value of feedstock [MJ/kg], ash [kg/year], water input and output [kg/year], SO_2 emissions [kg/year], H_2S emissions [kg/year], NO emissions [kg/year], NH_3 emissions [kg/year]
Temperature	°C	800 - 1000	8	
Pressure	bar	1 - 3	8	
Steam-to-biomass ratio	kg /kg	0.05 - 0.8	8	
Moisture	% mass	5.24 - 68.07	20	
Carbon content	% mass	40.46 - 84.98		
Hydrogen content	% mass	5.19 - 14.59		
Oxygen content	% mass	1.89 - 46.22		
Nitrogen content	% mass	0.16 - 3.21		
Chlorine content	% mass	0.06 - 1.05		
Sulfur content	% mass	0.03 - 0.62		
Pyrolysis				
Temperature	°C	400 - 750	10	Electricity consumption [kW], heat consumption [MJ], char production [kg/h], gas production [kg/h], oil production [kg/h], gasoline fraction, diesel fraction, wax fraction, C_1 in gas, C_2 in gas, C_3 in gas, C_4 in gas, CO_2 emissions [kg/h], CO emissions [kg/h], NO emissions [kg/h], NO_2 emissions [kg/h]
Vapor residence time	s	0.05 - 20.00	12	
Carbon content	% mass	65.86 - 84.98	18	
Hydrogen content	% mass	5.19 - 14.59		
Oxygen content	% mass	1.89 - 28.48		
Nitrogen content	% mass	0.16 - 1.65		
Chlorine content	% mass	0.05 - 1.05		

The system boundary included waste management processes (MRFs, incineration, biological treatments, gasification, etc.), recycling, final disposal in landfills, and the downstream utilization of the energy and materials supplied by the WMS, as depicted in Fig. 1.

A total of 15 categories were evaluated using Environmental Footprint 3.1 as the impact assessment method: global warming (100-year time horizon), acidification, terrestrial eutrophication, freshwater eutrophication, marine eutrophication, photochemical ozone formation, ozone depletion, human toxicity – cancer effects, human toxicity – noncancer effects, eco-toxicity, ionizing radiation, land use, water use, depletion of abiotic resources – fossil fuels, and depletion of abiotic resources – minerals and metals. Biogenic CO_2 emissions were not accounted for in the calculation of global warming.

2.5. Description of scenarios

A set of three scenarios was proposed in this study to demonstrate the applicability of the model for a system-level assessment. The scenarios represent the WMS of Madrid as an example of a large city making efforts in the collection and management of waste to meet legislation targets, comparable to many others across, and outside, the European Union (European Environment Agency, 2022).

- **Reference scenario.** The reference scenario represents a relatively modern WMS adapted with data from Madrid operating with the waste allocation factors described in Table 2. A key aspect of this system is that incineration is used to handle rejects and prevent a high landfill rate. In this scenario, the system generates energy-related products (electricity and biomethane) and materials (secondary materials and compost). The multifunctionality of the system was solved through the substitution approach, considering that each of the recovered products substitutes the corresponding market equivalents and the WMS was credited for the avoided environmental burdens. Electricity supplied to the grid was presumed to replace an equal amount of electricity generated by the Spanish electricity mix. Biomethane injected into the natural gas network replaces the production, distribution, and consumption of an equal volume of natural gas. Secondary materials were assumed to replace primary materials based on a substitution ratio. Additionally, the use of compost on land substitutes the production and application of mineral fertilizers, following a nutrient equivalence approach. This technology scenario corresponds to all processes connected by black lines in Fig. 1.
- **Realistic scenario.** Gasification and pyrolysis are implemented in the system with realistic expected capacities while incineration is removed from the system. Rejects are split evenly between these two technologies (i.e., 50 % of rejects go to each process). A downdraft gasifier operating at 900°C, 1.5 bar, and an equivalence ratio of 0.3 was selected for the assessment. The capacity of the unit was established at 116,000 tons of waste per year (Seo et al., 2018). Regarding the pyrolysis unit, the capacity was established at 100,000 tons per year. The pyrolysis reactor was set to operate at 500°C with 1 s vapor residence time. Biogas from the anaerobic digestor is directed to the DRM unit, where it is transformed into syngas and used for electricity production. The capacity of the DRM unit is also realistic, set at 15,341,632 Nm^3 of biogas per year. For the assessment, the DRM unit was configured to operate with cerium oxide as a catalyst at 900°C and 1 bar in the reactor. The syngas generated during the gasification and dry reforming processes was transformed into electricity to substitute electricity from the grid and the generated oil and char from pyrolysis were used to replace an equivalent amount of heavy fuel oil and charcoal based on the lower heating value. In this scenario, the technologies connected by colored lines in Fig. 1 were considered, and incineration was disregarded. Specific details on stream allocation can be consulted in Table 2, where the main differences in scenarios appear in the "Rejects from MRFs" and "Biogas" rows.
- **Unrestricted scenario.** All three new technologies (gasification, pyrolysis, and DRM) were implemented and distributed across the system in the same way as in the realistic scenario, but no capacity restrictions were set for the newly implemented processes. Details on stream allocation can be consulted in Table 2. Gasification and pyrolysis then have the necessary combined capacity to manage all rejects. In the same way as the previous scenario, the technologies connected by colored lines in Fig. 1 were considered, and incineration was disregarded. The main difference with the previous scenario is the capacity of the considered processes.

Table 2
Distribution of waste streams, biogas, and landfill gas across the individual processes (SS: source separated, MRFs: material recovery facilities; AD: anaerobic digestion; ICE: internal combustion engine). The values represent the percentage of the total stream allocated to each process.

Stream	Process	Reference	Realistic	Unrestricted
Packaging waste, SS	MRFs	100	100	100
Paper/ cardboard, SS	MRFs	100	100	100
Glass, SS	Transfer + MRFs	100	100	100
Organic waste, SS	AD	100	100	100
Residual waste, SS	MRFs / landfill	79/21	79/21	79/21
Recyclable materials	Recycling	100	100	100
Rejects from MRFs [a]	Incineration / gasification / pyrolysis / landfill	72/0/0/28	0/50 [e] /50 [e] /0	0/50/50/0
Organic waste, residual [b]	AD / composting / landfill	29/39/31	29/39/31	29/39/31
Rejects from AD	Landfill	100	100	100
Digestate [c]	Composting	–	–	–
Digestate (other)	Composting / landfill	64/36	64/36	64/36
Stabilized material	Landfill	100	100	100
Biogas [d]	Flare / upgrading / boiler / ICE / DRM	10/46.5/ 1.7/41.8/0	10/0/1.7/ 0/88.3	10/0/1.7/0/ 88.3
Landfill gas	Flare / ICE	98/2	98/2	98/2

[a] Rejects from sorting residual and packaging waste at MRFs.
[b] Organic waste separated from residual waste at MRFs.
[c] Digestate produced from source-separated organic waste.
[d] The allocation of biogas is calculated by the model as a function of capacity.
[e] The allocation of rejects going to gasification and pyrolysis in the realistic scenario is calculated by the model as a function of capacity.

Additionally, the above-mentioned scenarios were further divided into three source separation sub-scenarios (Low, Mid, High) to evaluate the combined impact of new technologies and increased waste separation on reducing landfill rates. For household waste, separation rates increase across Low, Mid, and High scenarios for each waste type: packaging waste (79.5 %, 80.0 %, 85.0 %), paper and cardboard (35.2 %, 70.0 %, 85.0 %), glass (60.2 %, 80.0 %, 90.0 %), and organic waste (42.3 %, 70.0 %, 85.0 %). In commercial waste, packaging waste, paper and cardboard, and glass remain at 0.0 % separation across all scenarios, while organic waste increases from 74.9 % in Low to 80.0 % in Mid and 85.0 % in High. Separation rates were selected using trend projections starting with data of 2019 (low separation) to meet separation targets for 2040 (high separation scenario) (Municipality of Madrid, 2019).

3. Results and discussion

The proposed methodology, which combines machine-learning surrogate models with MFA and LCA, constitutes an innovative result in itself. Beyond the methodological approach, the results derived from this study have been divided into two categories: process-level results, regarding the outcomes from process simulation for data generation and surrogate model training; and system-level results, regarding the outcomes from implementation and analysis of the WMS scenarios defined in Section 2.5.

3.1. Process-level results

As the interest of simulating does not lie in one particular case but in generating a wide range of valid data for the training of the surrogate model, pairplots of key process parameters were selected to illustrate the results. In Fig. 4, the triangle below the diagonal shows a scatter plot of all the resulting data points and the diagonal itself presents a histogram plot showing the frequency distribution of responses. The upper triangle depicts the probability density function of the dataset. As the datasets come directly from successful simulations runs in Aspen Plus, the data visualization in Fig. 4 represents intrinsic thermodynamic behavior that the machine-learning models have to incorporate.

Fig. 4a shows how the composition of the syngas varies across a sample of 6000 simulation runs dissagregated by type of gasifier. A set of two behaviors can be distinguished from the figure: the first one compiles all fluidized, updraft, and downdraft gasifiers (blue, pink, and orange points), while the second one englobes the circulating bed gasifiers. The first one presents relatively linear responses within similar numerical ranges. For instance, in the CO_2—CO scatter plot, a clear inverse linear relationship can be observed. The corresponding probability density function shows that, among all the gasifiers that present a linear trend, the updraft gasifier produces syngas with higher content in CO and CO_2. Similarly, H_2 and CH_4 also present clear correlation but more variables seem to be necessary to fully explain the behavior. Regarding the second behavior, circulating gasifiers show a much more dispersed response behavior around the sampled sensitivity area. For the CO_2—CO plot, this type of gasifier exhibits a nonlinear behavior. As the other variables were varied equally across the other gasifiers, this nonlinearity was directly attributed to the internal (more complex) recirculation of the fluidized bed present in this configuration and not in the others. In the case of gasification, other variables such as temperature or pressure in the gasifier also influence the response behavior, but only the type of gasifier was selected for simplicity in the visualization.

Fig. 4b shows the response behavior for the three produced phases (gas/oil/char) obtained from the pyrolysis process simulation for waste sources of varied carbon content at different temperatures. In this case, it can be observed that the higher the temperature, the higher the gas generation, compensated with lower generation of the liquid and solid products. Differentiated behaviors are a positive feature as they are more easily identified by the machine-learning models during the training procedure.

A similar plot corresponding to the process-level visualization for the dry reforming process can be found in the Supplementary Information. This includes a pairplot representing the response behavior of the produced syngas for the dry reforming process in three cases based on different catalysts. It shows a similar distribution across catalysts, thus making the composition of the generated syngas similar. Carbon monoxide exhibited a direct linear response behavior with hydrogen, an inverse linear response with methane, and a dispersed response with carbon dioxide.

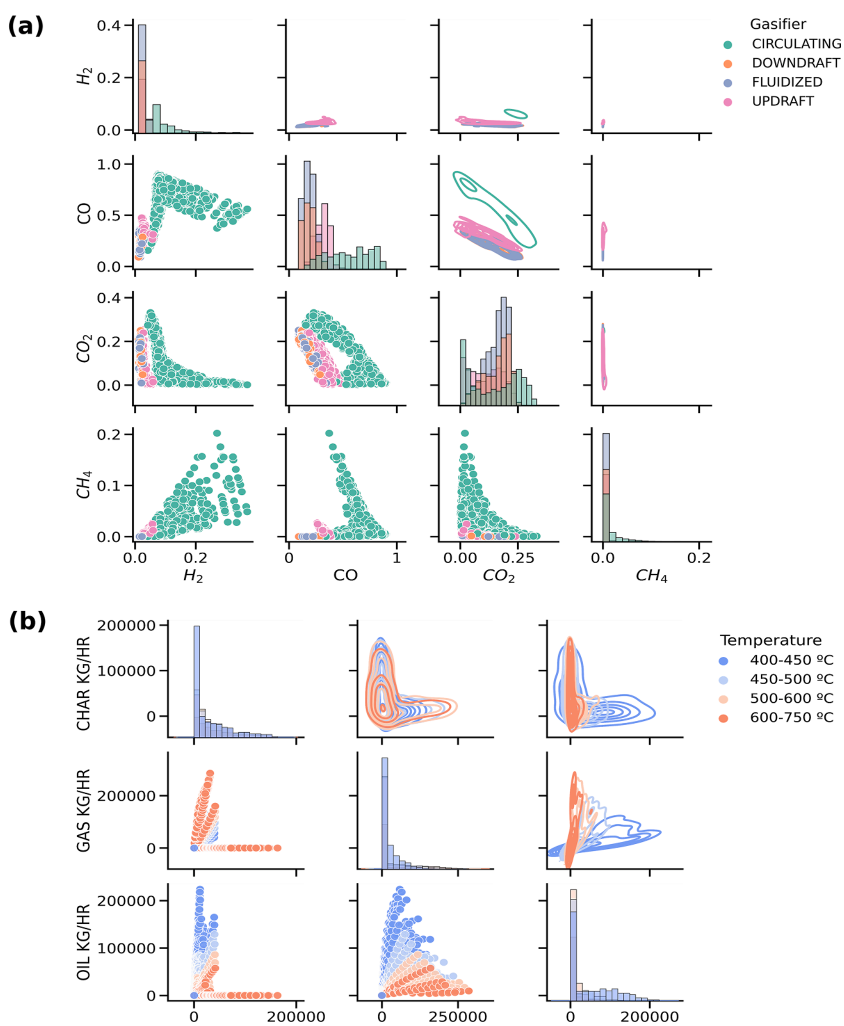

Fig. 4. Pairplots representing response behavior for (a) the composition of the generated syngas in the gasification process, and (b) the different product generations in the pyrolysis process for a range of operating temperatures.

These results are shown as an example of the trends and behaviors that are embedded in the trained machine-learning surrogate models. The waste management model is then capable to consider different operating conditions for the newly integrated processes. Furthermore, the model is capable of reflecting these changes in the generation of the LCIs used in the system-level LCA calculations.

3.2. System-level results

3.2.1. Life-cycle profile of the system

The global warming impact potentially generated by the WMS of Madrid over a year under the three assessed scenarios is presented in Fig. 5a. Results are shown for the lowest source separation rate sub-scenario, as it is the closest one to the current context in Madrid. Positive values indicate impacts generated by the system, while negative values represent avoided impacts from the generated products because of the substitution approach. The net value represents the difference between the generated and the avoided impacts.

In the reference scenario, the net global warming impact is 359.7 kt $CO_{2\text{-eq}}$. The main contributions at the process level came from landfilling and incineration: 267.3 kt $CO_{2\text{-eq}}$ and 194.3 kt $CO_{2\text{-eq}}$, respectively. The realistic scenario considers the replacement of the incinerator for a gasification unit and a pyrolysis unit with realistic capacities. In this case, the combined capacity of the units was not enough to manage all rejects, so a fraction of them were diverted to landfilling, thus increasing the global warming impact of this process. However, the net impact decreased compared to the reference scenario since both gasification and pyrolysis reversed their impacts by avoiding conventional market products (net impact of −10.6 and −83.2 kt $CO_{2\text{-eq}}$, respectively). The implementation of dry reforming decreased the total impact of anaerobic digestion, but its relative contribution to the system remained low. The unrestricted scenario shows the implementation of all of these emerging technologies without capacity restrictions, thus being able to manage all the rejects of the system and reducing the environmental impact of the landfill to a minimum of 235.4 kt $CO_{2\text{-eq}}$. As more rejects reach the pyrolysis and gasification units for processing, a greater substitution of products (electricity, pyrolysis char, and pyrolysis oil) occurs, which subsequently reduces the net global warming impact even further. The net impact becomes negative thanks to the implementation of these technologies, especially pyrolysis. A very slight improvement in the net impact could be associated with the unrestricted dry reforming unit compared to the second scenario.

The environmental characterization of the three assessed scenarios for a broader range of environmental indicators is presented in Fig. 5b. For each indicator in the figure, the impact for each scenario was relativized to the maximum absolute value in the category. Overall, the results show that implementing the emerging technologies entails an environmental performance improvement across all the studied indicators compared to the reference scenario. In addition to the global warming impact, terrestrial eutrophication, fresh water eutrophication, human toxicity – noncancer effects, ecotoxicity, and ionizing radiation impacts also became negative, indicating large co-benefits associated with emerging technologies. Other impact categories, including marine eutrophication and photochemical ozone formation, decreased by 75 % and 95 %.

The impact reduction is mainly associated with avoiding landfill and recovering products like oil and char from pyrolysis and electricity from gasification. However, the capacity of the new process units proved to be a relevant factor when enhancing environmental performance. The absolute values supporting Fig. 5 are provided in the Supplementary Information.

3.2.2. Landfill rate assessment

Fig. 6 illustrates the landfill rate results for each of the three analyzed scenarios and compares them to the 10 % target established in the Directive 2018/850 on the landfill of waste (European Commission,

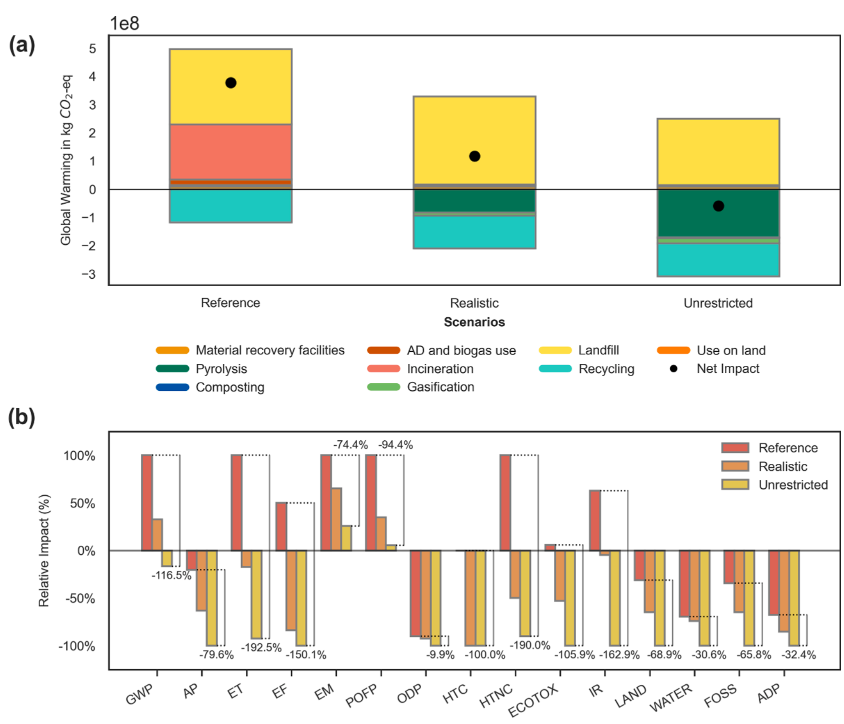

Fig. 5. (a) Annual global warming impact of the complete waste management system for the three assessed scenarios (black dots correspond to net global warming impacts), and (b) environmental comparison of the three scenarios for all studied impact categories (GWP: global warming; AP: acidification; ET: terrestrial eutrophication; EF: freshwater eutrophication; EM: marine eutrophication; POFP: photochemical ozone formation; ODP: ozone depletion; HTC: human toxicity – cancer effects; HTNC: human toxicity – noncancer effects; ECOTOX: eco-toxicity; IR: ionizing radiation; LAND: land use; WATER: water use: FOSS: depletion of abiotic resources – fossil fuels; ADP: depletion of abiotic resources – minerals and metals).

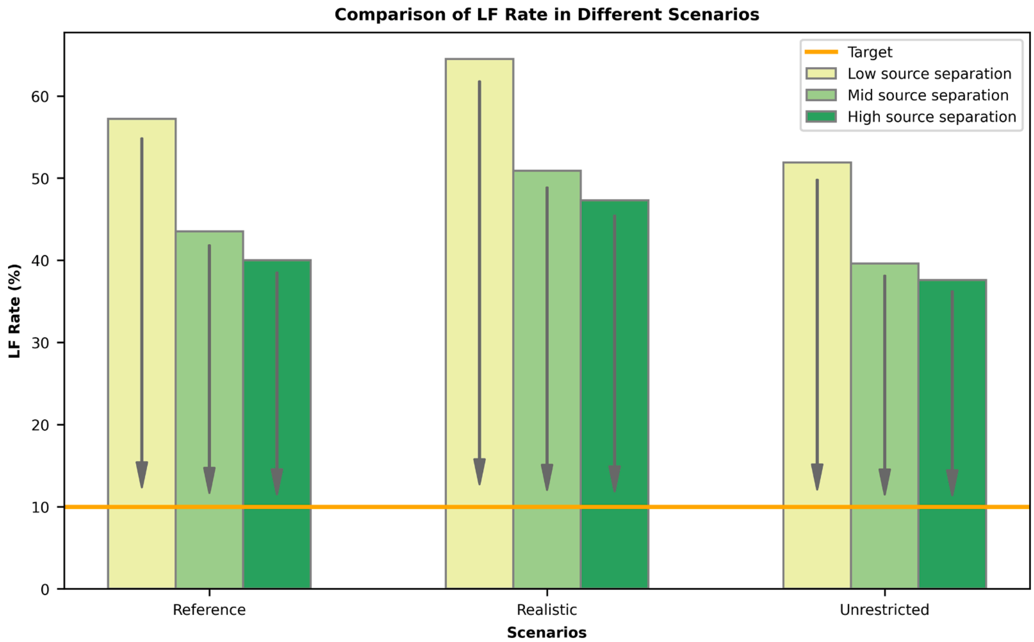

Fig. 6. Landfill (LF) rate for every scenario under different source separation rates (all scenarios are compared to the 10 % European target).

2018). Additionally, results from each scenario were contextualized considering three source separation rates (low, mid, and high, as specified in Section 2.5). The main factor affecting landfill rate is the capacity of the technology used to deal with rejects. The WMS generates 394,251 tons of rejects per year for the lowest source separation rate scenario. In the conventional scenario, incineration is used to manage these rejects while reaching the maximum capacity of the incinerator (328,000 tons of waste per year). The excess amount of waste is sent to landfill, leading to a landfill rate around 57 % for a system with low source separation (40 % for one with high source separation).

The realistic scenario contemplates the integration of both pyrolysis and gasification with realistic capacities (100,000 and 116,800 tons of waste, respectively). In this case, the total capacity to deal with rejects is decreased compared to the first scenario as these technologies are not yet found on the scale of large waste management incinerators. Consequently, the landfill rate for the second scenario with high source separation increased to 47 % as the untreated rejects would be diverted to landfill.

For the unrestricted scenario, no capacity limit was set for the pyrolysis and gasification processes, thus being able to deal with all rejects allocated to them. This led to a reduced landfill rate of 37.6 %, still far from the landfill target set by the European Commission. It should be noted that an equivalent landfill rate could be achieved with an equivalently sized incineration facility capable of managing all of the incoming rejects, although that would entail lower environmental benefits.

Adequate sizing of the technology used to deal with rejects from MRFs is key to reducing waste reaching landfills. For WMSs that have already achieved the landfill target through intense incineration and recycling, substituting the incinerator for a combination of pyrolysis and gasification could decrease the environmental impact, as shown in Section 3.2.1. However, in the case of systems that are still in efforts to reduce landfills, such as the one in Madrid, the mere implementation of these technologies might not be enough, even if source separation rates were increased.

The model can help identify the technological limits for landfill waste reduction, providing valuable insights for decision-making. Consequently, it can support claims demanding special efforts to increase social and business engagement to reduce waste generation. Additionally, when the operational management contract or the lifespan for an incineration plant nears termination, this model can help municipalities estimate the technical and environmental impacts of integrating emerging technologies into their system. Finally, a model like the one developed in this study would help estimate the required capacity of these new technologies for a given system. In the case study of Madrid, capacities of 197,125 tons per year would be required for both of these units, assuming each one deals with half of the generated rejects as in the studied scenarios.

In its reference configuration, the model represents a regional system with conventional technologies found in many WMSs across the globe. General findings regarding the substitution of an incineration plant for an emerging technology such as gasification or pyrolysis are applicable to systems relying on incineration to achieve a lower landfill rate.

4. Conclusions

In this study, emerging waste management technologies (pyrolysis, gasification, and dry reforming of methane) were integrated into an MFA and LCA model of a regional WMS. At the process level, machine-learning surrogate models were used instead of former approaches based on transfer coefficients. This approach enabled the simplified process models to retain the thermodynamic responsiveness of rigorous models. At the system level, the waste management model was useful in assessing the environmental impact of the illustrative system of Madrid under three different scenarios. Overall, the implementation of the above-mentioned technologies was concluded to involve a favorable impact on the environmental performance of the system. Gasification and pyrolysis were found especially interesting as their integration enabled the phase-out of the incineration unit. The assessment of the landfill rate of each scenario under different source separation rates showed that, despite the expected environmental benefits, the landfill rate reduction capacity of these emerging technologies was as limited as the one from incineration since all of them depend on their corresponding treatment capacities. The most optimistic scenario, with high source separation and no capacity restrictions for the new plants, achieved a landfill rate of 37.6 %. In this sense, if a system already has an acceptable landfill rate thanks to incineration, the substitution of an incineration unit for these new technologies would be environmentally beneficial while maintaining a low landfill rate. On the other hand, systems with incineration that do not achieve a low landfill rate would not reverse the situation by implementing these new technologies even though environmental impacts would generally be reduced. The most optimistic scenario showed a reduction of 116.5 % in terms of global warming potential and 10–193 % for other impact categories. In essence, optimizing the capacity of the existing and emerging facilities was concluded to be a key factor in minimizing both landfill rate and environmental impact. Finally, the economic analysis of the newly integrated processes and system optimization under environmental and economic criteria are proposed as future work toward a new generation of decision-making support models in the field of waste management.

CRediT authorship contribution statement

Nicolás Martínez-Ramón: Writing – original draft, Visualization, Methodology, Investigation, Formal analysis, Conceptualization, Writing – review & editing. **Robert Istrate:** Writing – review & editing, Methodology, Formal analysis. **Diego Iribarren:** Writing – review & editing, Supervision, Methodology, Formal analysis, Conceptualization. **Javier Dufour:** Writing – review & editing, Project administration, Funding acquisition.

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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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.rcradv.2025.200253.

Data availability

The data used in this research is available in the article (including supplementary information).

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