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EDITORIAL

Green and Circular Economy ECOMONDO 2020

23th International Trade Fair of Material & Energy Recovery and Sustainable Development

The papers collected in this special issue of *Environmental Engineering and Management Journal* were presented as lectures or posters at the scientific and technical conferences hosted by *Ecomondo 2020* held, given the pandemic, in the sole digital format from the Italian Exhibition Group headquarter in Rimini, Italy, during 3 - 6 November 2020 (http://en.ecomondo.com).

Ecomondo is the one of largest European exhibitions in the field of *Green and Circular Economy*, which, in the 2019 edition (before the pandemic), hosted over than 100,000 delegates from 60 different nations along with 1350 companies exhibiting their products and processes in 135,000 square meters. Despite the pandemic, *Ecomondo 2020* hosted over than 90 conferences and workshops, with extensive room dedicated to policies, research and innovation, innovation funding opportunities, education and training and international networking.

As with the previous editions, the aim of *Ecomondo 2020* was to explore recent industrial advances and opportunities in industrial technical waste production reduction, recycling and exploitation; sustainable agrifood and wood chains, biowaste collection and exploitation via integrated biorefinery schemes, with the production of biobased chemicals, materials and biofuels, including methane; industrial eco-design; industrial symbiosis, renewable and critical resources; water resources monitoring, protection and sustainable use in the civil and agrifood sectors; wastewater treatment and valorization with nutrients recovery and water reuse; marine resources protection and sustainable exploitation; sustainable remediation of contaminated sites, ports and marine ecosystems; indoor and outdoor air monitoring and clean up; and circular and smart cities.

Some of the international workshops were focused on the emerging trends in the in the circular economy domains and on the role of digitalization and industry 4.0 enabling technologies in process efficiency, eco-design and waste collection in the major industrial value chains. Some other workshops were focused on the technical and regulatory constrains currently affecting the implementation of circular economy value chains in the sectors of electronic and electric products, automotive, construction and demolition, packaging materials and textile and fashion. A special room has been dedicated to the recycling of plastic waste, biodegradable plastics and the monitoring, prevention and mitigation of marine litter. Finally, *Ecomondo 2020* also hosted a couple of events on the priorities of the Mediterranean macro-region, and in particular the water scarcity of the area, the Mediterranean Sea contamination (also due to marine litter) and its sustainable exploitation.

Ecomondo 2020 hosted about 90 conferences, more than 700 oral communications and almost 100 papers. This special issue contains some of such papers and provides some of the key information presented and discussed in the frame of some of the most relevant technical and scientific conferences of 2020 edition of *Ecomondo*.

We believe that this collection of papers will be useful to people who could not follow the digital edition of *Ecomondo 2020*. It is primarily towards them but it also aspires to provide permanent records in the promotion, adoption and implementation of the major priorities and opportunities of the green and circular economy in Europe and in the Mediterranean basin, with the conversion of some of the key local environmental challenges into new opportunities for a green and sustainable growth of the areas mentioned.

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Guest Editor:
Fabio Fava, PhD, Professor, *Alma Mater Studiorum - Università di Bologna*, Bologna, Italy

Fabio Fava, born in 1963, is Full Professor of "Industrial & Environmental Biotechnology" at the School of Engineering of University of Bologna since 2005.
F. Fava published about 250 scientific papers, 180 of which on medium/high IF peer-review international journals of industrial and environmental biotechnology and circular bioeconomy. He has 8680 overall citations, a h-index of 55 and an i10 index of 145 (Google Scholar) along with 180 papers quoted by Scopus. He is actively working in the fields of environmental, industrial and marine biotechnology and of the circular bioeconomy in the frame of a number of national projects and collaborative projects funded by the European Commission. Among the latter, he coordinated the FP7 collaborative projects NAMASTE, on the integrated exploitation of citrus and cereal processing byproducts with the production of food ingredients and new food products, and BIOCLEAN, aiming at the development of biotechnological processes and strategies for the biodegradation and the tailored depolymerization of wastes from the major oil-deriving plastics, both in terrestrial and marine habitats. He also coordinated the Unit of the University of Bologna who participated in the FP7 collaborative projects ECOBIOCAP, ROUTES, MINOTAURUS, WATER4CROPS, ULIXES and KILL SPILL.
F. Fava served and is serving several national, European and international panels, by covering, among others, the following positions:
• Member of the Scientific Committee of the European Environmental Agency (EEA), Copenaghen, for the "Circular economy and resource use" domain (2021-);
• Italian Representative in the "European Bioeconomy Policy Forum" and the "European Bioeconomy Policy Support Facility" of the European Commission (2020-);
• Italian Representative in the Horizon2020 Programme Committee of Societal Challenge 2: European Bioeconomy Challenges: Food Security, Sustainable Agriculture and Forestry, Marine, Maritime and inland water research" (European Commission, DG RTD) (2013-);
• Italian Representative in the "States Representatives Group" (SRG) of the Public Private Partnership "Biobased Industry" (PPP BBI JU) (Brussels) (2014-); he is chairing the SRG since October 2018;
• Italian Representative in the BLUEMED WG of the EURO-MED Group of Senior Officials (EU Commission DG RTD and Union for Mediterranean) (2017-);
• Italian Representative in the initiative on sustainable development of the blue economy in the western Mediterranean the "Western Mediterranean Initiative" WEST MED, promoted by the EU Commission (DG MARE) in close cooperation with 10 countries of the area (2016-);
• Italian Representative in the "Working Party on Biotechnology, Nanotechnology and Converging Technologies" of the Organization for Economic Co-operation and Development (OECD, Paris) (2008-);
• Chair (2011-2013) and currently Deputy Chair of the "Environmental Biotechnology Section" of European Federation of Biotechnology (EFB) (2013-).
Finally, he is the scientific coordinator of the International Exhibition on Green and Circular economy ECOMONDO held yearly in Rimini (Italy)

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COGENERATION MANAGEMENT SYSTEMS IN PUBLIC AND PRIVATE SECTOR: SECOND CIRCULAR FINANCE MODEL

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Abstract

The Italian context is currently characterized by an economic crisis and by the need to eco-innovate the production and management processes of the same. In this situation it is necessary to implement development strategies that do not increase the debt in the state budget and local authorities. To achieve this goal, as for the cogenerate energy processes with the same amount of resource, various forms of energy are produced (electricity, heat, steam) thus maximizing the results. For the financial and economic processes there is a strategy that leads to the same amount of resources used to maximize results. The public sector through the National Recovery and Resilience Plan (NRRP) and the Ministry of Economic Development (MISE) supports the eco-innovative and resilient development processes through incentives, tax reliefs, grants.

The NRRP speaks of resilience, in this context the biological concept of self-pity is introduced, a system that continually redefines itself and is sustained and reproduced from within by applying it to the economic and financial system of the country.

In this paper, the second model of circular finance is introduced and explained a model that starting from the integrated planning of economic variables of the public and private sectors identifies the system economies able in the medium and long term, through the economic benefits derived, to self-finance the industrial eco-innovative processes of a Country. In short, the process of industrial sustainability is self-financing through the benefits arising from the system.

Key words: circular finance, circular economy, cogeneration, eco-innovation, financial cogeneration, public-private management

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1. Introduction

Starting from public accounting, state budget and budgets of local authorities, identifying the budget items, variables, both intended as expenses related to the safeguarding and protection of the environment and expenses related to incentives, tax reliefs, grants (Milano et al., 2015). By identifying the variables relating to the private sector, production costs, environmental protection costs, costs linked to industrial eco-innovation for the transition from a linear to a circular economy.

Industry today must eco-innovate in order to be competitive (UN, 2015). According to the European Union's definition of eco-innovation: "The key to Europe's future competitiveness (UNEP, 2015).

Eco-innovation means any innovation that results in significant progress towards the goal of sustainable development by reducing the impacts of our production methods on the environment, strengthening nature's resilience to environmental pressures, or enabling a more efficient and responsible use of natural resources (UNEP, 2016).

Eco-innovation also represents an opportunity for companies because it leads to lower costs, helps to seize new growth opportunities and improves the company's image in the eyes of consumers (European Commission 2015). In addition, the search for new industrial eco-innovation processes leads to greater process knowledge, production of innovative materials, thus greater know-how in process management and chemical management, and greater system flexibility (European Commission, 2019).

In order to eco-innovate production processes, variables to the public sector, budget expenditures, budget expenditures for environmental protection and protection (waste management, environmental damage management for examples) (Donida et al., 2015). By placing the economic determinants of the public and private sectors within the same system, it is possible to obtain intersectoral system economies capable of generating value autonomously.

In many cases, the implementation of an innovative eco-process by the private sector can result in decreased spending by the public sector. Systemic economies can thus be achieved in this context. The joint management of the economic and financial budgets of the public and private sectors leads to the identification and enjoyment of these economies and thus have benefits for society as a whole.

The intersectoral matrix of cogeneration management generates system economies that can give rise to a state of system self-financing or circular finance. This document proposes a strategy for managing intersectoral matrices called: ”**Integrated public and private sector cogeneration system**”. System consisting of three subsystems: private sector, public sector, environment, Fig.1.

2. Variables of a complex cogeneration system

In order to maximize the benefits of an integrated public-private system, and therefore to maximize system economies, it is necessary to identify the determining variables of the complex system. With this aim, the potential common targets of the two spheres public sector and private sector are identified. In order to maximize the benefits of an integrated public-private system, and therefore to maximize system economies, it is necessary to identify the determining variables of the complex system. With this aim, the potential common targets of the two spheres public sector and private sector are identified. Integrated management thus leads to greater efficiency and effectiveness of administrative action (as required by the Public Function).

Therefore, it leads to maximization in the achievement of targets with maximization of economic performances (lower costs, lower expenses, higher derived revenues, maximization of management performance) and natural ones (energy and matter) with consequent lower environmental impacts. Fig. 2 shows the structure of the two spheres.

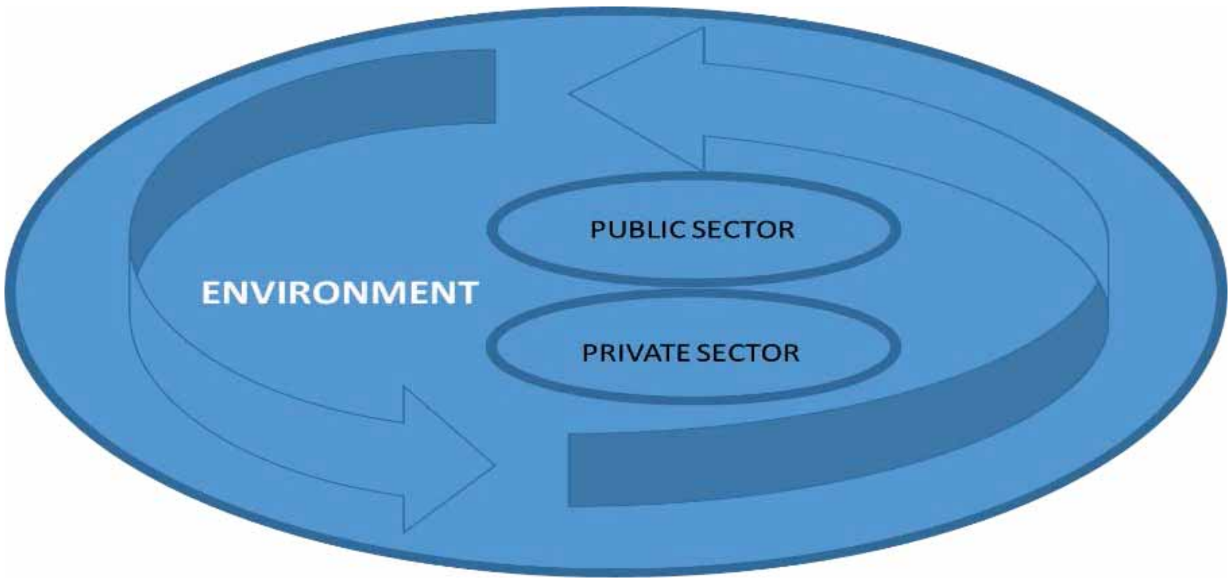

Fig. 1. Integrated cogeneration management

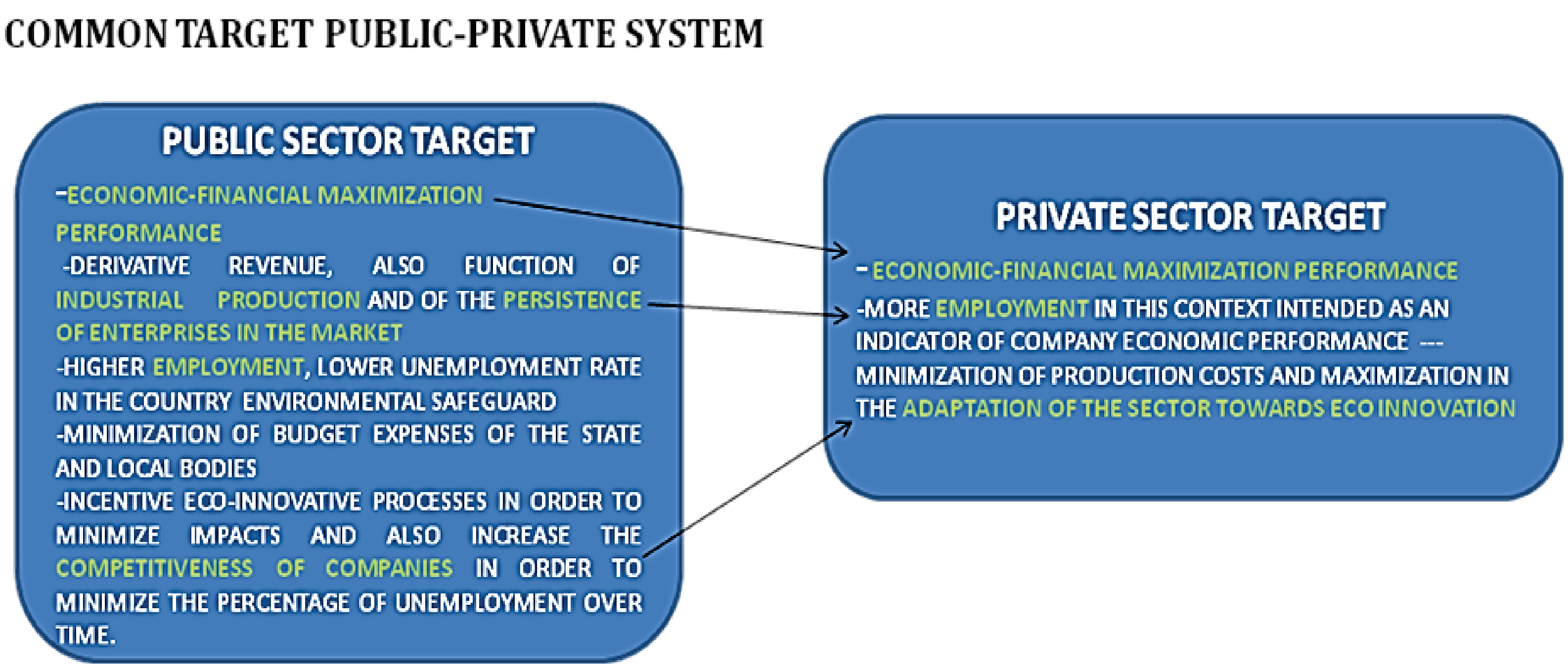

Fig. 2. Target public-private sector

By putting the two sectors, public and private, into a system, we can find the determining variables that must be evaluated in the choice of eco-innovative projects that should also be financed with public funds, therefore through contributions and tax relief. Thus, financing in a timely and determined manner only some private projects, those that also generate benefits in the public sphere, in the form of lower expenses in the budget of the State and public bodies and public administrations, thus continuing this assistance in the medium and long term. For example, the revamping with LED lamps instead of incandescent or halogen lamps used for public lighting generates energy savings in the long term and less maintenance of the equipment. Therefore, an initial investment to replace traditional lamps with LED ones is amortized on average in one year of operation, therefore the capital invested is reinstated in one year and subsequently we will have lower energy consumption and therefore savings in budgetary expenses for public administrations for the private sector a gain from the execution of the project and for the environment a saving on the impacts generated by the lower production of energy for lighting.

Cogeneration management between the public and private sectors consists of planning eco-innovative processes jointly, evaluating the economic and financial variables of the two sectors jointly. Through cogenerated management, thus defined, public-private system economies can be maximized to the point that an eco-innovative project can be financed by the future benefits (decrease in costs for the public sector, and decrease in expenses for the private sector) related to its implementation.

As energy cogeneration refers to the combined production of electricity and heat, public-private cogeneration management tends to increase the benefits of the system. From the implementation of an eco-innovative process, on the one hand the public sector can benefit by reducing future expenses related to environmental management and protection, and on the other hand the private sector can benefit economically (lower production costs, product differentiation, etc.).

Through the derived (derives from the compulsory withdrawal of wealth by the state from private individuals.) revenues, the State acquires the economic resources necessary to encourage eco-innovative processes in the public sector. By selecting only, the projects, to be incentivized-financed, that is, those that lead to public-private system benefits (which determine a reduction in public spending in the medium and long term) creates self-cogenerated, process that are self-fueling. For example, the budget of the Municipality of Rome in 2020 shows that expenditure on 'Sustainable development and protection of the territory and the environment' amounted to €1.360.290.569, or €479.43 per person (Rome Municipality, 2020).

From this evidence one can understand how important the government's investment process is and how public expenditure is used. From this evidence it is possible to understand how important the government's investment process is and how public expenditure is used, both for the public and private sectors, and for the citizen.

In particular, taking as a reference the expenses related to environmental protection, enhancement and recovery and the expenses related to waste we can imagine that if the Municipality financed even partially projects that lead to a reduction of these expenditure items, part or all of the invested capital would recover from future expenses not incurred. For example, if the Municipality of Rome financed only the eco-innovative projects that lead to a reduction in such expenses, these projects could have a good degree of self-financing from the private public system.

The Municipality of Rome by financing certain projects that comply with the rules that credit institutions follow for the self-sustainability of an investment. Specifically, credit institutions finance only projects that lead to an internal rate of return on invested capital, in the form of a loan, higher than the opportunity cost which is given by the rate of return that would be obtained by investing in the current average securities and real estate sector. In order to calculate this IRR, the Municipality should also include the sum of the expenses not incurred in the future budget. For example, if the Municipality granted a non-repayable grant to companies, for example equal to 10 M €, which treat waste and the recycling of such waste, resulting in lower future expenses in the Municipality's budget, due to the non-management of this part of the waste, there would be an indirect recovery of the investment. If the expenses not incurred were equal to 0.5 M € per year in 5 years, for example, there would be a self-financing rate of 25% and an IRR of 5%.

The public sector through the proceeds deriving from derived revenues (taxation from the private sector) grants incentives to companies, private sector. In the planning phase, eco-innovative projects of private companies should be encouraged, which tend to reduce public spending by the state and local public bodies in order to obtain system economies and therefore the tendency towards system self-financing. Fig. 3 shows the technique of the public-private cogeneration management system, the benefits of the public sector, reduction of expenses, compensate for the incentives given by the State to companies.

Therefore, planning and identification of eco-innovative projects according to this method leads in the medium and long term to make the investment process of the public and private sectors more efficient (Tanese et al., 2006). Thus, creating greater employment stability, greater penetration of companies in the market, increase in derived revenues, greater know-how of companies, thus bringing the national financial system to economic and financial autopoiesis, a system that continuously redefines itself and sustains and reproduces itself own internal.

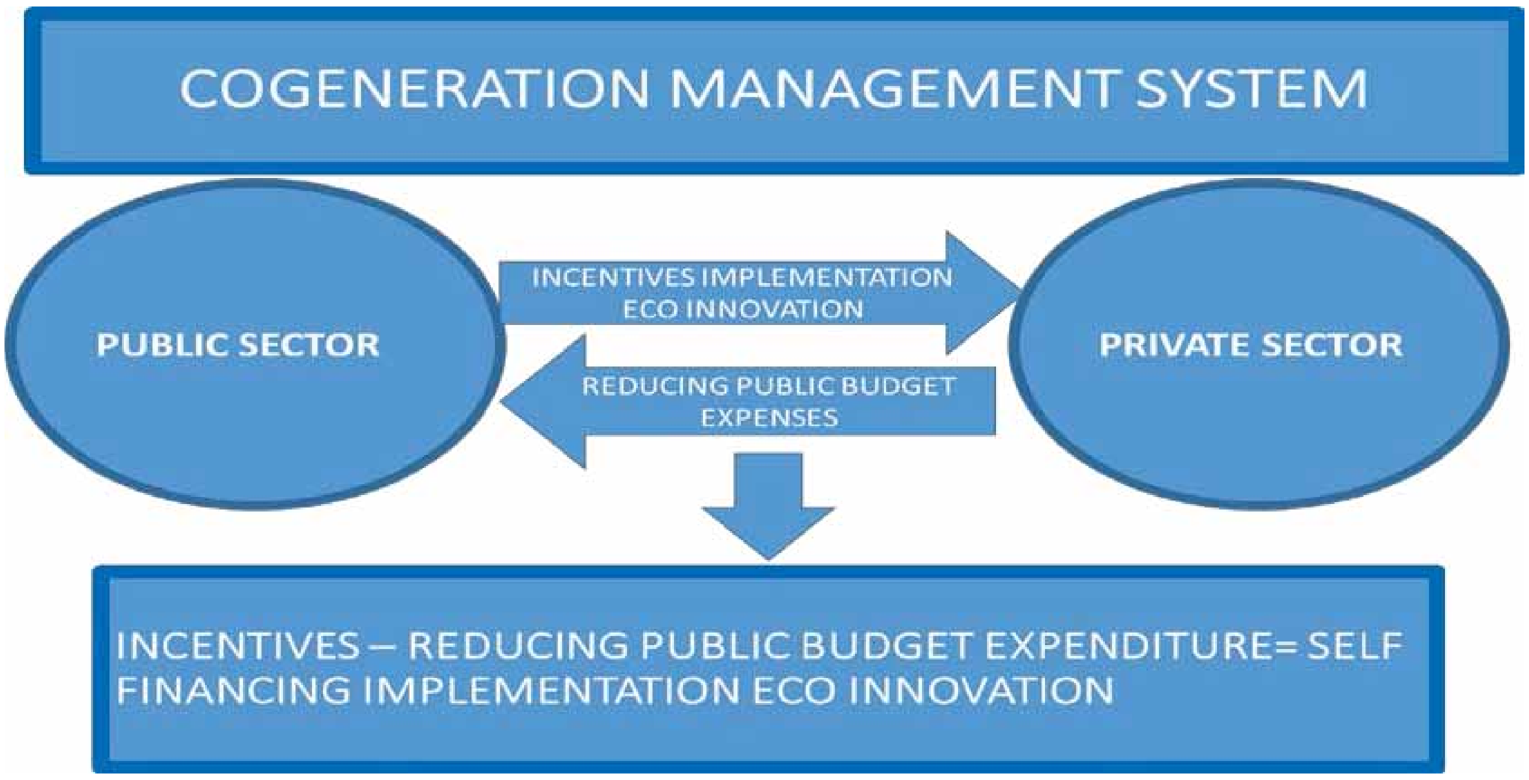

Fig. 3. Cogeneration management system

Initially we go to calculate the sum of all the benefits of public and private sector system resulting from the integrated management of the two spheres. Subsequently, by equalizing the initial investment to zero, we can obtain the interest rate that sets it at zero. In this case the investment is self-financed by future benefits, a state of total circular finance. When the interest rate thus obtained is equal to or greater than the opportunity cost (opportunity cost is the average interest rate that would be obtained by investing in the current securities and real estate market), banks consider the eco-innovative investment profitable and are willing to finance it.

Second circular finance model: mathematical model relating to the application of the concepts of circular finance (Eqs. 1-2):

$$NPV = \sum_{t=1}^{T} \frac{F\ public\ expenses\ reduction}{(1+i)^t} + \frac{F\ private\ sector\ benefits\ endogenous}{(1+i)^t} \tag{1}$$

$$I_0 = \sum_{t=1}^{T} \frac{F\ public\ expenses\ reduction}{(1+i)^t} + \frac{F\ private\ sector\ benefits\ endogenous}{(1+i)^t} \tag{2}$$

If $I_0=0;\ i \geq C_0$

Setting the initial investment I_0 equal to zero, we obtain the interest rate as a function of the time that leads to the total self-financing of the investment. If the discount rate that brings I_o equal to zero is equal to or greater than the opportunity cost (C_0) the investment is attractive for credit institutions. According to this logic, the State, by implementing this model to establish which investments to make or not, to which eco-innovative projects to contribute, could reduce the public debt and trigger a virtuous process that leads the private public system to economic and financial **autopoietism**.

Just as autopoiesis in biological systems, it can be seen as a network of constraints that work to maintain themselves, in the same way joint management between the public and private sectors leads to maximizing system economies and thus financially self-sustaining eco-innovative processes.

3. Circular finance techniques for the cogeneration system (public and private sector)

The concept of circular finance is based on the logic that an eco-innovative process can be financed by the future benefits of implementing the same. To achieve this goal, systemic benefits must be maximized. It is precisely through the joint management of the public and private sectors that economies of scale can be created that can increase the benefits.

The circular finance techniques for the cogeneration system (public and private sector) to follow to reach an autopoietic state of the system are:

1. plan circular finance strategy, implementing the second mathematical model of circular finance;
2. evaluation of private projects to be encouraged by the public sector on the basis of paradigms related to circular finance;
3. in a certain territory identification of system economies, contemporary public-private benefit;
4. in a certain territory identification of environmental criticalities o opportunity;
5. control: territorial strategic plans identified by the various actors present in the area.

The Italian Federative Association of Consulting Companies stated that "strategic planning allows to promote an intensification of the relationships existing between actors of the local system who recognize and share the same development objectives". The Department of Public Function states: "The Local Authority must voluntarily decide to play an active role in the economic and social regeneration of the territory (Pisano et al., 2012; Sáez-Martínez et al., 2014) assuming the leadership role of the mobilization and coordination process of local actors, in the construction and implementation of a shared development vision." The TSP Territorial Strategic Plan already exists. In this context, with the collaboration of all the actors active in the area, the activities to be implemented are planned.

Almost all Italian municipalities have the TSP, it would be desirable if not necessary that the local public authorities evaluate the private projects to be financed with public contributions through the second circular economy model described in the previous chapter. In the following we will describe the projects that respond to the concept of system self-financing, circular finance.

The Macrolotto of Prato (Iraldo et al., 2011) was in a territorial situation in which the aquifer tended to resource depletion. In this context, the industrial district with the help of the Municipality has implemented a consortium for the purification of water thus avoiding the withdrawal of the aquifer, Fig. 4.

Fig. 4. Water purification Consortium CONSER Prato's district

Private individuals (Macrolotto di Prato) have had benefits as if the water table continued to be, resource depletion they would have been forced to supply water through tankers with consequent large costs.

The Municipality would have had enormous economic damage deriving from the depletion and loss of the water resource. So, public and private have decided to create this water purification consortium, the Municipality has disbursed € 300.000/year, a cost item passed on to the companies that continue to use groundwater. In this way, 5M/m^3 of groundwater per year was saved, equal to 125.000 (Tanese at al., 2006). There are many examples of eco-innovative projects that have led to system self-financing, where all the actors involved have benefited without burdening the state coffers and local public bodies. The technique lies in framing the criticality to be remedied or the opportunity that can generate the implementation of an eco-innovative process-system, through the business plan of the project it is possible to determine the future cash flows generated and the expenses avoided. By discounting the avoided flows and expenses, the interest rate generated is determined by placing the investment at zero time equal to zero. Once the interest rate has been determined, it is compared with the opportunity cost (rate deriving from an average investment or real estate at time zero).

The more a project determines a high internal rate of return, the greater the amount of self-financing of the system, the greater the attractiveness of credit institutions to lend capital, the greater the convenience also for the public sector to finance the project since in the medium and long term will generate value. With this technique an environmental problem of depletion of the aquifer has been solved without affecting the public sector coffers. Everyone benefited from it.

Many techniques of this type lead to system self-sustainability, circular finance. Other examples are the redevelopment of brownfields, soils polluted by disused industrial processes are redeveloped by private individuals or the public sector, thus generating value by reclaiming the territory and following the directives of the European Union regarding the objective of "consumption of new land equal zero before 2050".

4. Conclusions

In the context of the National Recovery and Resilience Plan (NRRP), this article proposes the second circular finance model. By incorporating public and private sector variables into the same system, financial resources are maximised by creating self-sustaining value, similar to autopoiesis in biology.

The system feeds itself from within, leading to greater independence from external financial sources. By assessing and selecting the projects that the public government should support, the system is economically and financially self-sustaining. The public sector can thus encourage eco-innovative projects without burdening the government coffers, thus generating value.

The public sector thus assumes a function of partial control of public and private investment. All actors benefit, the private sector by innovating, the public sector by increasing revenue derived, creating jobs and increasing employment stability, generating even more procedural know-how for both. The necessary tools are a territorial strategic plan that identifies projects that lead to self-financing, also reducing future public sector expenditure.

The Territorial Strategic Plan (STP) is already present in the territories and can be a valid tool to bring together all the actors in the territory and to implement the mathematical model of circular finance in this specific document that allows public administrations to identify the projects that create more value in the public sector than in the private sector. In this way, by incentivising projects that produce greater system economies, a cogeneration system is created that from an initial vector generates value in several economic spheres, as in the energy sector from an energy vector with cogeneration there is the joint production of various products (electricity, steam, heat, other).

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PRELIMINARY STUDY ON VALORIZATION OF SCRAPS FROM THE EXTRACTION OF VOLCANIC MINERALS

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Abstract

Powders < 3mm of pumice and lapillus (quarry scraps of national volcanic minerals) were employed in the tailoring and characterization (from the physical, chemical and mechanical point of view) of geo-polymers and lightweight aggregates.
Geo-polymers were obtained at room temperature by substituting 70 - 80 wt% of metakaolin by volcanic scraps and employing an alkaline solution with a Na_2SiO_3/NaOH ratio from 0.8 to 1 for pumice and lapillus series, respectively. Within 24 h and in water, bulk specimens resulted with good integrity, with pH values around 9-11 and conductivity increasing over time, but less for the lapillus-containing sample richest in metakaolin indicating more compactness. The porosity, ranging around 32-33% for all the samples, increased up to 45% for the formulation based on 80% of lapillus. The best mechanical performance was achieved by lapillus samples: compressive strength in the range 35-38 MPa against 6-8 MPa of pumice ones.
Lightweight aggregates were created by powder sintering at 1000 °C for 1 hour of 85 wt% of volcanic scraps and 15 wt% of spent coffee grounds used as pouring agent. Additional formulations were realized adding 50 wt% of nourishing mixture P and K-containing in the form of animal bone meal and vegetable biomass ashes. The specimens resulted porous and light (porosity around 60%), with good capacity of water retains, and, except in two cases, with neutral pH and conductivity values below 2 mS/cm, indicating a possible use for substrate (growing layer) in roof gardens, green roofs, house gardens, etc..

Key words: geo-polymers, lightweight aggregates, quarry scraps, recycling

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1. Introduction

The recycling of waste materials and residues is an important objective recognized at the regulatory level in the circular economy. As written by Stephen Hinton "The aim of the circular economy is to retain and recycle technical nutrients in the economy, to cycle biological nutrients from the economy to the biosphere and back, and to utilize money to facilitate transactions and trade". In particular, while plant and animal material coming from the ecosystem return to it after being degraded (returning nutrients to the environment), metal, plastic glass components and any other kind of residue represent parts of material or new raw material for other refurbished or created products (acquiring a new value) (EMF, 2017). This last aspect, important for those countries, such as Italy, poor in raw materials, has positive economic and job repercussions, but always with a view to environmental protection.

Construction sector, ceramics and cement factories are large users of primary raw materials from natural resources (clay, quartz, kaolin, feldspar, limestone, etc.) with a consequent negative

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environmental impact (impoverishment of the territory, climate change, transport cost, etc.) so they have increased their effort to implement secondary raw materials use.

It is known that the conventional building construction consumes not renewable resources, generates waste and emitters greenhouse gases (Górecki et al., 2019). Thus, was born the context of sustainable construction with the aim of limiting the impact of this commercial sector on the environment. This new context brings new challenges about sustainable construction methods, but also great benefits too. These include lower operating costs, so it appears that the use of the latest sustainable technologies in construction processes could potentially provide significant savings of € 410 billion per year on global energy spending (BAB, 2019). Direct savings are also available to construction companies: by reducing waste, for example, would will reduce the fees charged by company waste management, adopting more efficient vehicles, will save on fuel costs. Another benefit is represented by the fact that sustainable construction can help the company's reputation by demonstrating a sense of corporate social responsibility. Precisely this can also be associated with the use of recycled raw materials to realize products that, in their turn, contribute to environmental certifications such as LEED (Leadership in Energy and Environmental Design) and BREEAM (British Research Environmental Assessment Method) certifications. The tools to limit the impact of this production sector on the environment include a greater exploitation of renewable and recyclable sources, a saving in energy consumption, always taking care to create healthy and environmentally friendly environments.

Moreover, the attention to new materials development with specific performances, also covering niche or expanding sectors, is of great interest for the productive compart. Among the materials with very interesting potentialities and which can good tolerate the presence of recycling fractions we find geo-polymers and lightweight aggregates.

Geo-polymers are a class of materials that can be defined as hydraulic binders produced starting from powders, mainly alumino-silicate, which are dissolved in a highly alkaline environment. These materials can be considered “ceramics consolidated by alkaline reaction”, meaning that they can be produced using a chemical reaction and not a thermal sintering, ultimately leading to the same chemical-physical and mechanical properties typical of ceramics (Leonelli et al., 2013). The prefix geo- indicates that we are talking about a product of geo-synthetic, that is, a product that mimics materials already present in nature; the suffix -polymer instead refers to the production process (geo-polymerization), that is a polymerization by poly-condensation. In 1978 the French chemist Joseph Davidovits used for the first time the definition of "geo-polymer" to indicate in general materials based on alkaline alumino-silicates, which are obtained by condensation and subsequent polymerization. More generally as a subset of the family of alkali activated materials, inorganic binders derived from the reaction of an alkali metal salt with a silicate powder. More specifically as a subset of inorganic polymers, characterized by the highest content of aluminum and sodium and by the amorphous or semi-crystalline microstructure and greater cross-linking of the silicate chains. Geo-polymers, whether used pure or with fillers or reinforced, already find applications in many fields of industry from metallurgical, polymers and civil to waste treatment, restoration, biomaterials (Medri, 2009).

Lightweight aggregates (LWAs) are granular materials, manufactured with both natural materials, and by-products or recycled source materials, having particle densities not exceeding 2000 kg/m^3 or loose bulk densities not exceeding 1200 kg/m^3 for use in concrete and mortar according to UNI EN 13055: 2016. Other applications cover civil engineering, geotechnics or agriculture. LWAs can be divided into natural and artificial. Among the former, pumice is widely used (with very modest mechanical resistance to compression), while among the latter are very common: expanded clays, expanded clayey schists, vermiculite and perlite. The principle on which the preparation of these artificial aggregates is based basically consists in bringing the raw product to a sufficiently high temperature (1000-1300°C), such as to cause the elimination of gaseous substances, while the simultaneous formation of an appropriate quantity of liquid phase promotes sintering of the grains while maintaining a good number of cavities in the material. Expanded clay usually comes in the form of porous, light and very resistant balls, produced by firing various types of clay at high temperatures. Inside there is a porous core that gives lightness and allows liquids to be absorbed and drained, to maintain the right humidity in the environment in which it is inserted, as well as acting as a thermal and acoustic insulator. It also has a high mechanical resistance to compression, is a natural product and does not release toxic substances or particles and fibers. Anyway, a certain amount of thermal energy is requested during the expansion process.

Porous minerals useful for making lightened products are pumice and lapillus. These are naturally expanded volcanic minerals. Their natural expansion is caused by the acid gases dissolved in the lavas which, released suddenly, cause the material to swell. During the rapid cooling phase, the resulting solid which is not totally crystallized has alveolar cavities produced by the imprisonment of the aforementioned gases inside the rock. The chemical composition of the pumice’s magma with an average amount of SiO_2 of 56 wt% causes a high viscosity of itself and the rapid cooling hinders the gases escape, originating a rock structure with several little pores intercommunicating with each other and also externally (Fig. 1a). Instead, the magma that generated volcanic lapillus has a lower SiO_2 content, around 49 wt%, which lowers the viscosity of the lava. This associated to a slower cooling, facilitate the escape of a certain amount of gases present within the magma. In the end, the lapillus obtained will have a lower percentage of pores than the pumice, but with larger sizes (Fig. 1b). Finally, the color difference between the two minerals, white and red for pumice and lapillus respectively, are imputable to a higher amount of Fe_2O_3 present in the second (on average 9 wt% against 4 wt%).

Although these inert volcanic minerals find applications in sectors such as nursery gardening (cultivation substrates and moulds, cultivation outside of the ground, full field), green areas (sports fields, green car parking areas, hanging gardens, ornamental meadows), green roofs, building industry (lightened concretes, plasters, thermal insulation, acoustic insulation, construction of light items, fume outlets, light fillings, biological building industry), dentistry (dried pumice for polishing and whitening of natural teeth), their mining activity produces residues. The fine fraction (<3mm) of the pumice and lapillus quarrying activity extracted in Italy and which is stored in the same quarry area, do not find an adequate marketing and involves additional costs and charges. Indeed, if used as quarry restoration, the scraps have the additional cost of transport from the plant to the quarry (on average 0.6 € / m^3), if piled up in areas of competence of the quarry (authorized as internal landfill) and then resold, are subjected to a regional tax of 0.30 € / m^3 (Lazio).

Bibliography exist on the recovery of waste from mining operations and other raw materials as result from a recent report showing that such waste is usually reprocessed with comminution and enrichment techniques that allow to obtain: valuable raw materials (metals in particular), minerals of industrial utility (quartz, kaolin for example) and residues useful for the rehabilitation of the site are (Salmine et al., 2019). Similar information does not seem to exist for scraps from the extraction of volcanic minerals. With these premises and with the aim to define new marketing sectors, this work deals with the engineering and preliminary characterization of prototypes of geopolymers and lightweight aggregates based on the fine fractions of the volcanic inerts above described. Briefly:

1) geopolymers, alkaline activated materials or cold-consolidated aluminosilicate materials by alkaline activation (substitution of metakaolin up to 90%) in which the presence of volcanic minerals allows to obtain promising porous and lightened geopolymers in the field of internal and / or external panels with possible applications in acoustic and thermal insulation. Volcanic minerals are suitable for alkali activation due to their high amorphous fraction formed as a result of rapid cooling during volcanic activity.

2) lightweight aggregates, i.e. materials with inert mineral matrix, with low specific weight, in which the clay components have been completely replaced with these scraps, exploiting their high content of silica (49-57%) and alumina (18-19%), and obtained by fast heat treatment (1000 °C, 1 hour). The addition in the formulation of a post-consumer product with an organic matrix (spent coffee grounds) which develops gas at the consolidation temperature, has allowed the creation of porosity. The material was then functionalized with a view to "fertilizer material" bringing two of the three main fertilizer’s nutrients: P as animal bone meal ash and K as vegetable biomass ash.

From the results obtained seem that lightweight aggregates have good perspective to lighten and fertilize the soil, in particular for the pH, conductivity and porosity point of view. This is a good starting point, to be deepened, for outdoor applications as green roof or vertical forest (with a view to modern and "sustainable" architecture) and indoor cultivations (a niche sector which is however expanding).

Geopolymers represent another interesting perspective: the presence of volcanic minerals leads to particularly porous and lightened matrices compared to those based on metakaolin with other interesting properties, therefore perspectives in the construction sector (ARPAV, 2007).


(a)


(b)

Fig. 1. Pumice (a) (http://www.europomice.com/products/pumice/) and Lapillus (b) (http://www.europomice.com/product/lapillus/)

2. Materials and methods

2.1. Raw materials choice and characterization

The volcanic raw materials such as pumice and lapillus were supplied by Europomice Srl that took care natural volcanic minerals currently extracted from four quarries located near Grosseto and Viterbo (area of Lake Bolsena). The excavation of this type of minerals provided a commercial grain size material and another amount characterized by grain size below 3-4 mm which remains mainly unexploited.

Volcanic raw materials were dried at 100 °C in an oven for 24 hours in order to remove the moisture. Subsequently, they were ground and sieved under 75 μm to bring the granulometry closer to that of the main component of geo-polymers, i.e. metakaolin (MK) Argical 100 (supplied by BAL-Co and with a grain size < 80 μm).

Spent coffee grounds (SCGs), a post-consumer product, were dried in the same way of volcanic scraps. The inorganic fraction is negligible, while the organic one prevails, as can be seen from the weight loss around 98% and with a carbon contribution of 50% by weight. Precisely for this reason it was decided to use this residue as a pore forming agent during the firing of the aggregates. Potassium which is a nutrient element was supplied by a vegetable biomass ash, while phosphorous by animal bone meal ash resulting from the calcination (900 °C) of the flour. Flour is already used as a fertilizer in organic agriculture but also as a natural supplement for feeding livestock thanks to the phosphorus content present in the composition.

Chemical analyses of volcanic raw materials and metakaolin were performed by X-Ray fluorescence and provided by the themselves raw materials supplier companies, while those of spent coffee grounds, biomass ash and bone meal ash were performed by the same technique using XRF Thermo Scientific Model ARL PERFORM'X, software OXSAS. In order to investigate the crystalline phases into the raw materials, mineralogical analysis was carried out using an automatic diffractometer X-Pert PRO, Panalytical, with Ni-filtered Cu Kα radiation; the patterns were collected on the powdered samples, characterized by a size less to 38μm, in the 5-70° 2θ range (step size 0.02° and 1s counting time for each step). Moreover, quantitative mineralogical analysis of volcanic materials was given by Europomice Srl.

The alkaline attack test, used to determine the reactive fraction, allowed to verify the reactivity of the two volcanic minerals to obtain geo-polymers (Ruiz-Santaquiteria et al., 2011). One gram of volcanic materials was immersed in 100 mL of 8 M NaOH solution (solid/liquid ratio of 1/100) in stirring condition for 5 hours at 80 ± 2 °C (Ruiz-Santaquiteria et al., 2011). The final solution was filtered in order to separate the liquid and solid fraction.

The liquid fraction was acidified by HNO_3 to pH=2 in order to perform ICP/OES (VARIAN LIBERTY AX) to quantify the amount of Si and Al in the leachate (Lancellotti et al., 2013).

2.2. Geopolymers preparation

Pumice, lapillus and metakaolin were used as aluminosilicate-based materials. Na_2SiO_3 (SiO2/Na2O=3) solution and NaOH 8M solution were used as alkali activator by mixing in a ratio of 1:1.25 or 1:1 for pumice or lapillus-containing formulations, respectively.

In details the steps of preparation:
- volcanic ash powders and metakaolin were mixed;
- a mixture of alkaline solutions sodium hydroxide-sodium silicate was used to obtain a viscous paste;
- the paste was manually mixed for 5 min;
- the paste was poured into a plastic mold.

Curing conditions: the samples were closed inside a plastic bag for all curing time at in order to avoid air exposure and maintain a constant moisture level.

Curing time: 28 days

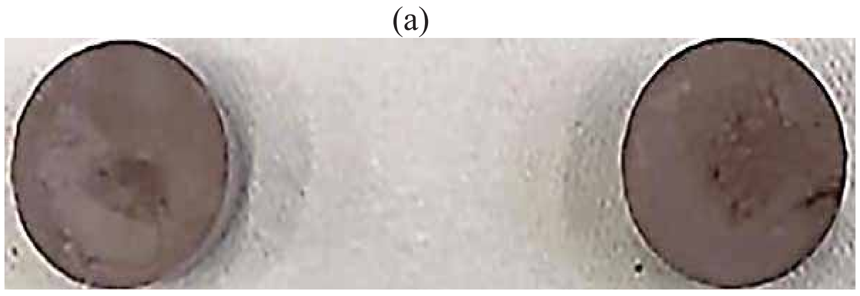
Curing temperature: room temperature (25 +/- 3°C)

The protection of the sample from the air was necessary to avoid the formation of a layer of sodium carbonate on its surface. This phenomenon was due to the low reaction rate of pumice and lapillus with alkaline solution during the reticulation phase of the geo-polymers. The characterizations of the specimens took place at a curing time of 28 days.

In this research two different series of samples were prepared; the first based on pumice instead the second based on lapillus. Both of them were characterized by the addition of metakaolin in order to optimize the aluminum content, because volcanic materials are poor of Al.

- FIRST SERIES: Alkali Activated Materials (AAMs) based on 70-80 wt% of pumice and 20-30 wt% of metakaolin (MK) (Fig. 2a and Table 1);
- SECOND SERIES: Alkali Activated Materials (AAMs) based on 70-80 wt% of lapillus and 20-30 wt% of metakaolin (MK) (Fig. 2b and Table 1).

(a)



(b)

Fig. 2. Pumice AAMs at 28 curing days (a) and lapillus AAMs at 28 curing days (b)

Table 1. Formulations of Series 1 and Series 2 samples (MK: Metakaolin; P: Pumice; L: Lapillus)

Sample	*MK (g)*	*Pumice (g)*	*Lapillus (g)*	*NaOH (mL)*	*Na_2SiO_3 (mL)*	*Alkali ratio Na_2SiO_3/ NaOH*	*H_2O (g)*
P70	30	70	\	20	16	0.8	4
P80	20	80	\	20	16	0.8	4
L70	30	\	70	20	20	1.0	\
L80	20	\	80	20	20	1.0	\

2.3. Lightweight aggregate preparation

Four compositions were tailored based on volcanic raw materials and spent coffee grounds only or added of 50 wt% with a nourishing mixture (41% pumice + 25% vegetable biomass ash + 34% animal bone meal ash) prepared by dry-mixing in a slow ball mill for 30 min in order to give fertilizer properties, as reported in Table 2.

Table 2. Lightweight aggregates batch compositions

Sample / Raw material (wt%)	*P*	*P/L*	*P 1*	*P/L 1*
Pumice	85	42.5	85	42.5
Lapillus	-	42.5	-	42.5
Spent coffee grounds	15	15	15	15
Nourishing mixture	-	-	50	50

Spherical samples of aggregates about 1.5-2 g in weight were made by manual palletization using the prepared mixtures. To obtain a good plasticity needed for shaping, the powdered mixtures were moistened with an adequate water content (20-30% wt%) in order to avoid the formation of cracks. After drying in an oven at 105 ± 5 °C for at least 24 hours, in order to remove free water in the mixture to avoid possible cracking of the aggregates during firing due to sudden evaporation, the samples were inserted in an electric oven at 1000 °C for one hour. When inserted, the kiln was already hot and this is done in order to simulate the thermal shock that the aggregates undergo during industrial processes which, however, generally occur at higher temperatures (from 1200 to 1400 °C).

2.4. Geo-polymers characterization

Geo-polymers characterization was performed from chemical, physical and mechanical point of view. The samples at 28 days of curing were immersed in distilled water with solid/liquid ratio of 1/100 at room temperature for 24 hours in order to investigate the chemical stability and the compactness of their structure. This integrity test provided a qualitative evaluation on the stability of the matrix after 24 hours (Kiventera et al., 2018).

Further, the material's chemical stability in aqueous environment was monitored by pH and ionic conductivity measurements. A bulk sample was placed in distilled water (solid/liquid ratio wt% was 1/10) and stirred for 24 hours at room temperature. pH (Laboratory PH sensor Hamilton type Liq-glass SL, OAKTON Eutech Instruments pH 5/6 and Ion 6) and conductivity (OAKTON Eutech Instruments CON 6/TDS 6) were measured at different times, such as 0, 15, 30, 60, 120, 240, 360, 1440 min in order to analyze the release of the ions in the solution during the 24 hours (Finocchiaro et al., 2020; Lancellotti et al., 2013, Lancellotti et al 2015).

To obtain quantitative information on the microstructure of alkali-activated materials and their lightness characteristics, the total porosity percentage (TP (%)) was obtained by processing absolute (Mycrometrics Accupyc 1340), and apparent (Enveloped Density Micrometrics Geopyc 1360) density data, indicated as ρ_{abs} and ρ_{app}, using Eq. (1):

$$TP(\%) = \frac{\rho abs - \rho app}{\rho abs} \cdot 100 \qquad (1)$$

Finally, mechanical compressive test was performed on the specimens after 28 curing days at room temperature. Four samples of each composition in cubic form with a side of 2 cm were subjected to compressive test according to the standard UNI EN 826 (Barone et al., 2020) employing an Instron 5567 Universal Testing Machine with 30 kN load limits and displacement of 3 mm/min.

2.5. Lightweight aggregates characterization

To analyze the weight variation of the aggregates during firing (water, organic matter, carbonates, etc.) a weight loss test was performed. This procedure was a preliminary test to check the stability and the preliminary resistance of the matrix (Andreola et al., 2019). Firstly, the specimen was dried and weighed (Wi), then this one was weighted after the firing (Wf); so, the weight loss percentage (WL (%)) was determined by Eq. (2):

$$WL(\%) = \frac{W_i - W_f}{W_i} \cdot 100 \qquad (2)$$

In order to investigate the capacity of water retain, very important characteristic in gardening applications, the water absorption was determined. This parameter is related to the open porosity. The measure was conducted according to the standard EN ISO 772-21:2011. The specimen was immersed in distilled water in static condition for 24 hours at room temperature. The sample, after drying, was weighted before (W_i - initial weight) and after (Wf - final weight) the immersion in water. Water absorption percentage (WA (%)) was quantified using Eq. (3):

$$WA(\%) = \frac{Wf - W_i}{W_i} \cdot 100 \qquad (3)$$

The total porosity was calculated by Equation 1 from the absolute and apparent densities measured with the same procedure described in 2.4 paragraph. pH and electrical conductivity measurements were carried out as reported in UNI EN 13037:2012 (pH rule standard) and UNI EN 13038:2012 (conductivity rule standard). The content of the soluble salts in the soil should be controlled because of their excess could lead to a serious plant imbalance as well as a pH different from neutrality could cause serious problems.

Bulk specimens (10 g) were placed in distilled water with solid/liquid ratio as 1:5 in stirring condition (360 rpm) for 1 hour at room temperature. The liquid was filtered in order to obtain a transparent liquid fraction; on this eluate pH and electric conductivity were measured.

3. Results and discussion

3.1. Raw materials characterization

Chemical data of raw materials as pumice, lapillus, metakaolin, spent coffee grounds, biomass and bone meal ashes are shown in Table 3. Volcanic mineral scraps were suitable to form a silico-aluminate matrix both for geo-polymers and lightweight aggregates.

The high Loss of Ignition of SCGs underlined the presence of organic compounds (fatty acids, amino acids, polyphenols and polysaccharides as referred in Andreola et al 2019) and confirmed by the elemental analysis (%): 2.39 N, 50.28 C, 6.99 H, 0.08 S and 38.54 O suitable to induce porosity during aggregates firing. Finally, vegetable biomass and animal bone meal ashes were considered as nutrient supplier mainly of potassium and phosphorous, respectively. For geo-polymers the content of SiO_2+Al_2O_3 is important together with the amorphous fraction in order to have optimized alkali activation. The SiO_2+Al_2O_3 of pumice was equal to 75.2% while for lapillus was 67.4%. These two parameters allow to hypothesize that pumice could be a more suitable material for alkali activation. Furthermore, Table 3 shows the presence of small percentage of Ba, Sr, Zr and Mn in volcanic materials.

The quantitative information about the mineralogical composition of pumice and lapillus is reported in Table 4. Since pumice contains 79.7% of amorphous phase while lapillus 11%, the former was considered a more suitable material to make AAMs as discussed above. Both raw materials contained Sanidine (K,Na)(Si,Al)$_4$O$_8$, Anorthite $CaAl_2Si_2O_8$, Analcime $NaAlSi_2O_6(H_2O)$, Hematite Fe_2O_3 and other crystalline phases in smaller percentage as reported in Table 4.

The engineering of geo-polymeric materials went from a pre-screening to determine the reactive fraction in terms of Si and Al ions released in alkaline environment being known that a Si/Al mass ratio between 2 and 3 is associated to materials with a 3D rigid network, suitable for a cement, concrete (Lancellotti et al.2013). Table 5 shows Si/Al mass ratios very similar for both volcanic materials, compared with the ratio of metakaolin.

Pumice shows higher release values for both Si and Al, in agreement with the higher amorphous fraction detected by XRD. Both ratios for volcanic materials are higher with respect to metakaolin, probably due to the less amount and solubility of Al in these materials.

Table 3. Chemical composition (wt%) of raw materials used

Oxide	*Pumice*	*Lapillus*	*Metakaolin*	*Spent coffe grounds*	*Vegetable biomass ash*	*Animal bone meal ash*
SiO_2	56.6	49.1	58.97	0.01	1.57	0.43
Al_2O_3	18.6	18.3	34.70	\	0.37	0.02
Fe_2O_3	3.94	9.15	1.40	0.02	1.13	0.01
TiO_2	0.54	1.08	1.30	\	\	\
CaO	3.06	9.27	0.10	0.24	5.78	53.89
MgO	1.17	4.25	0.10	0.09	0.54	1.11
Na_2O	1.98	2.35	0.10	0.06	0.56	1.40
K_2O	8.55	3.66	0.70	0.89	59.81	0.04
P_2O_5	0.13	0.45	\	0.16	1.46	41.24
Mn_3O_4	0.13	0.14	\	\	\	\
BaO	\	0.09	\	\	\	\
SrO	\	0.11	\	\	\	\
ZrO_2	0.07	1	\	\	\	\
SO_3	0.13	\	\	0.06	4.99	\
Cl	\	\	\	0.01	6.77	\
LOI	4.84	1.44	2.63	98.11	16.60	1.00

Table 4. Quantitative mineralogical analyses (wt%) of Pumice and Lapillus

Mineralogical phase	*Pumice*	*Lapillus*
Amorphous	79.7	11.0
Quartz **SiO_2**	1.1	\
Sandino **$(K,Na)(Si,Al)_4O_8$**	11.2	19.8
Anothite **$CaAl_2Si_2O_8$**	3.0	26.1
Analcime **$NaAlSi_2O_6(H_2O)$**	7.2	13.2
Diopside **$CaMgSi_2O_6$**	0.3	2.1
Muscovite **$KAl_2(Si_3Al)O_{10}(OH,F)_2$**	1.5	1.2
Hematite **Fe_2O_3**	8.8	4.5
Plagioclasio **$(Na,Ca)(Si,Al)_4O_8$**	3.1	6.9

Table 5. Si and Al release in NaOH 8M at 80 °C detected by ICP-OES

Element (mg/L)	*Pumice (mg/L)*	*Lapillus (mg/L)*	*Metakaolin*
Al	491	134	316
Si	1063	309	594
Si/Al	2.16	2.31	1.89

The error associated to the measurement is up to 20%

3.2. Geopolymers characterization

All the compositions, submitted to integrity test in water for 24 h, resulted unchanged confirming the efficacy of the geo-polymerization process and the compactness of the matrix. Monitoring of pH and conductivity in aqueous environment and at established times and temperature allowed to evaluate the crosslinking of the sample network and the geo-polymerization reaction.

The first series of samples (Fig.3a), characterized by the presence of pumice, showed a value of pH that increases during 24 h for P80 (from 8.70 to 10.23), instead for P70 samples the pH values follow a constant trend from 9.60 to 10.02 in 24 h. For both formulations P80 and P70 the conductivity measurements increased during 24 h from 12.4 to 280 mS/m due to the ions release in the solution but Fig. 3a show no significance variation between the two formulations. This means that a higher amount of metakaolin into the matrix (from 20 to 30%) didn't involve reinforcement of the matrix and better chemical stability. The pH of the second series, containing lapillus, showed a constant trend for both formulations L80 and L70 during 24 h (from 10.2 to 10.01). This mean that a higher amount of metakaolin produced a more compact and stable sample in aqueous environment confirmed by reduction of released ions within the solution. The pH and conductivity measurements are characterized respectively by an error of 2% and 8%.

The total porosity (TP %), calculated by elaborating the experimental density values according to Eq. (1), was studied to confirm the light weighting nature of pumice and lapillus.

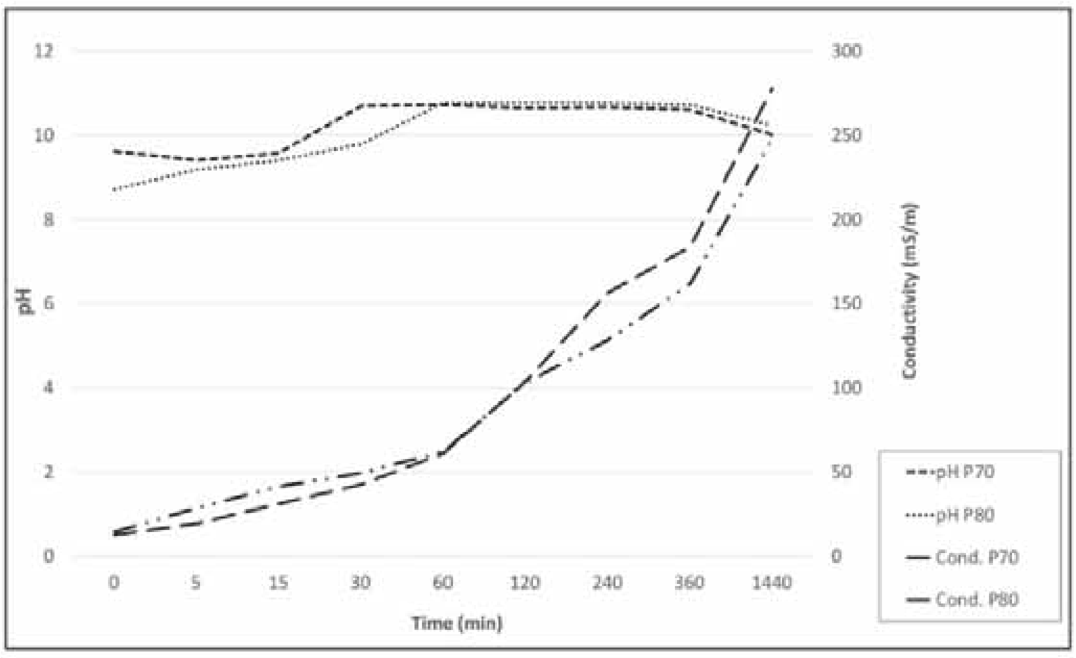
Looking at Fig. 4, it appears evident that the amount of volcanic mineral (80 or 70%) and the consequent amount of metakaolin (20 and 30%) is irrelevant within pumice-containing geo-polymers, and almost the same value of TP% was calculated for 70% of lapillus-containing sample. A material more porous and lightweight was obtained with 80% of lapillus and 20% of metakaolin, reaching a TP% around 45% instead of a mean of 32% for the other specimens.

In order to investigate the mechanical properties of the pumice and lapillus specimens and the comparison between the two series, the compressive analysis was carried out. Fig. 5 shows that lapillus samples were characterized by the best results in terms of compressive strength (38MPa) with respect to pumice ones (6MPa) and these values are really similar to metakaolin geopolymer reported as standard. The amount of metakaolin inside the compositions does not show appreciable effect, for both the series. The results show the higher performance of lapillus sample with respect of pumice one due to the increase of geo-polymerization reaction and the dissolution of lapillus particles under the effect of alkali activators.

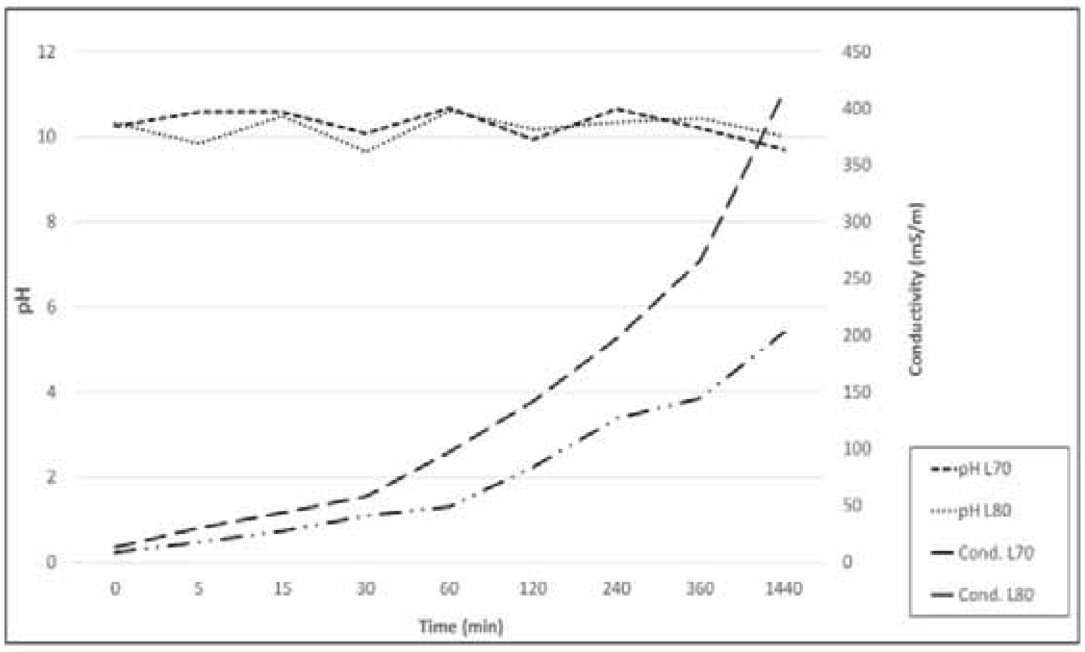
Data obtained are supported by bibliography. Values from 32 to 38 MPa were obtained by Barone et al. 2020 on geo-polymeric specimens 75 wt% volcanic ash and 25 wt% metakaolin-containing and with 28 curing days. Dener et al. 2021 working on alkali activated blast furnace slag/Portland cement composite using 80, 70 and 60% lightweight pumice aggregate by volume of total aggregate obtained the highest values ranging from about 18 to 22 MPa and 8 to 13 MPa for specimens 60 and 80 wt% of pumice content, respectively.

The reductions in compressive strength were more evident when the pumice aggregate content was increased from 70% to 80%. Values of compressive strength around 40MPa were also find by Jaya et al. (2020) for metakaolin-based geopolymers with alkali ratio 0-8-1.0 as for geopolymers prepared in this research.

Higher compressive strength (from 55 MPa for 3 days' age to 65 MPa for 90 days' age) values were found by Karatas et al. (2019) for blend produced with entirely kaolin, but in this case with a Na_2SiO_3/ NaOH ratio of 3, higher than the ratios used in this research (0.8 and 1).



(a)



(b)

Fig. 3. pH and conductivity of pumice-containing samples vs. time (a) and of volcanic lapillus-containing samples in function of time (b)

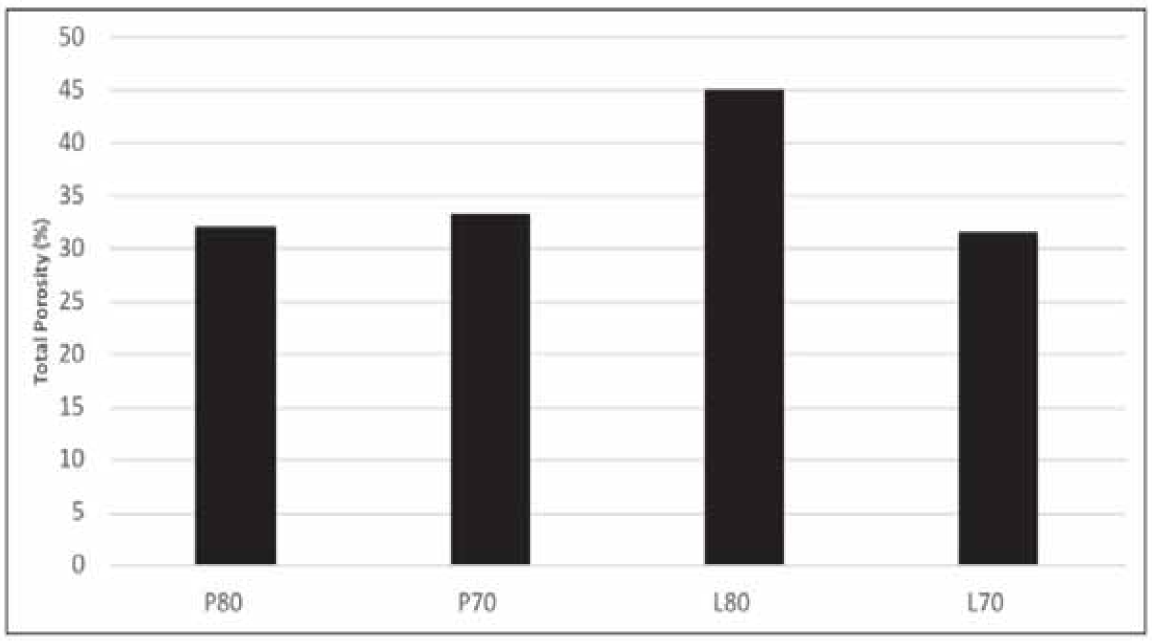


Fig. 4. Total porosity percentage of pumice and volcanic lapillus-containing samples

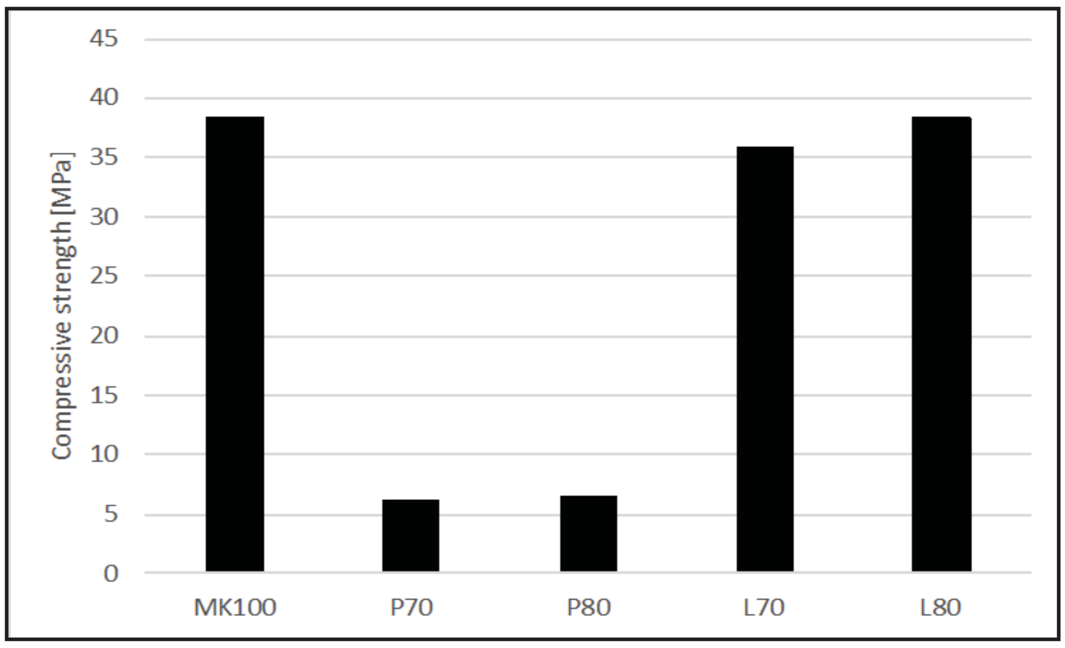


Fig. 5. Compressive strength of pumice (P70-P80), lapillus (L70-L80) samples and the reference specimen MK100 (Metakaolin 100%)

3.3. Lightweight aggregates characterization

In this study, the authors completely replaced the red clay used in the LAWs composition reported in previous paper (Barbi et al., 2020), maintaining the ratio of components mineral /porous agent 85/15. The optimization of the SCGs amount was studied in Andreola et al. (2019). All compositions characterized, were codified indicating the volcanic mineral matrix P: total pumice and P/L: matrix composed in equal amount of pumice and lapillus. For completing the mixture, the 15 wt% of SCGs as pore forming agent was added. These compositions can act as draining medium in the green roof. The compositions named P1 and P/L1 correspond to the above matrix described with the addition of 50 wt% of a nourishing mixture containing two kinds of agro-ashes which provide the main nutrients (P and K) for the vegetal culture. These compositions were tailored with the aim of using them as fertilizer.

Physical features of the aggregates were measured in order to verify the feasibility to use the volcanic scraps as alternative raw materials. The weight loss (WL %) allows to appreciate the lightness of the specimens after firing. The values calculated are around a range from 15 to 20% for all specimens, except the P / L composition which has a high value. The WL% is associated to the loss of free water necessary for the paste preparation (~20-25%), organic compounds decomposition (from SCGs) and carbonates decomposition (from animal bone meal ash).

The UNI EN 13055:2016 rule specifies that an aggregate is considered as Lightweight Aggregate (LWA) when the particle density is lower than 2.00 g/cm^3. Table 6 shows that all analyzed samples complied with the limit required for the standard. The aggregates containing only the matrix resulted lighter respect to those containing also the agro-ashes. The density is particularly important factor for the use of materials as a drainage component in layers of green roofs (formulations with only volcanic mineral scraps) and, again, as a light substrate, with fertilizing properties (aggregates formulations with nutrients). Regarding the absolute density values, they derived from the components into the formulation. In fact, the P/L compositions show a greater density respect to the P ones (density of pumice = 0.5-0.6 g/cm^3; density of lapillus = 1.05-1.15 g/cm^3 (EuroPomice, 2018; EuroPomice, 2019). Besides, the presence of agro-ashes increases the absolute density values. In summary, the aggregates obtained are effectively porous and light, the calculated total porosity is around 60% for all compositions tested (Table 6).

Finally, the water absorption, strictly related to the open porosity, is an important factor to choose the aggregate‘s application. From the Fig. 6 it can be observed that P/L sample showed the highest WA% values, P1 and P/L1 show intermediate values and P composition resulted with the lowest value indicating a high sintering degree.

Concerning the chemical properties, pH and electrical conductivity were measured on the filtered liquid after contact with the aggregates. The pH of the soil measures the concentration of hydrogen ions in the circulating solution, i.e. the liquid phase found in the spaces left free between the particles of the solid fraction (clay, sand and silt). Its value depends of the kind of ions present (alkali or not). This chemical parameter greatly influences the microbiological activity (responsible of the breaking down organic matter), the availability of mineral elements and the adaptability of the various plant species. The pH of the soil also influences the solubility of the various mineral elements in the solution of the soil both from the decomposition of the minerals of origin and from the fertilizers distributed, determining their accumulation in forms more or less available for the plants or their leaching towards the lower layers deep. In general, the best pH condition of the soil for the development of crops is around neutrality (pH between 6.5 and 7.5): in a neutral environment the nutrients in solubilisation phenomena are in fact reduced or absent, the supply of mineral elements is generally more balanced and microbiological activity is favoured. Soils that have a pH below 5.5 generally are characterized by low percentage of calcium, magnesium, and phosphorus and in these conditions the solubility is high for aluminium, iron, and boron, while is low for molybdenum (USDA, 1998). Based on these considerations, lightweight aggregates should have a pH as close as possible to neutrality. The data reported in Fig. 7 show that all the samples meet the conditions of neutral pH, with a slight overshoot towards the alkalinity only of the pumice-based aggregate (7.7).

Another fundamental parameter to be monitored is electrical conductivity. The soluble salts present in the soil (coming from the soil, groundwater or irrigation water, fertilizers) are essential for plant nutrition, but their concentration must be contained within certain values. For crops, the range corresponds to values greater than 0.2 mS/cm and less than 2 mS/cm. High salt concentrations can cause nutritional imbalances, toxic effects on plants, damage to the soil structure and, in some cases, changes in pH. Apart from these extreme situations, an increase in salinity generally determines an increase in the driving force of the circulating solution which in turn causes greater difficulty in absorbing water and mineral elements by plants: this phenomenon depends not so much on the salt content soluble, but by the osmotic pressure exerted by them.

Although electrical conductivity, E.C., provide no direct measurement of specific ions or salt compounds, it has been correlated to concentrations of ions such as nitrates, potassium, sodium, chloride, sulphate, and ammonia (USDA, 2006). As far as conductivity is concerned, it is noted that only the composition based on pumice and lapillus (P/L1) with the addition of 50% of nutrients exceeds the threshold value of 2 mS/cm, therefore it could only be suitable for more resistant crops. The conductivity values of the other compositions fall within the reference range. It is possible to observe that the compositions without nutrients show very low values (Fig. 8). These results indicate the ease of release of the ions present in the ashes at the pH of use.

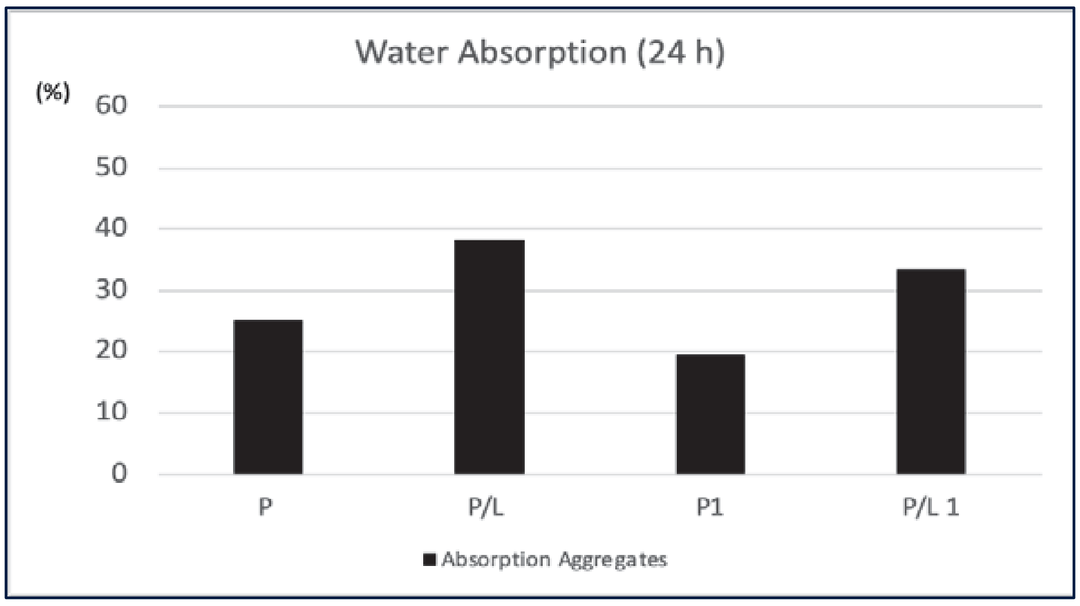


Fig. 6. 24h-inmersion water absorption of the prepared aggregates

Table 6. Physical properties of the lightweight aggregates

Sample code	***Absolute density (g/cm³) (standard deviation)***	***Apparent density (g/cm³) (standard deviation)***	***Total porosity (%)***
P	2.1913±0.0016	0.9953±0.0043	59
P/L	2.5650±0.0015	0.9609±0.0018	63
P 1	2.9820±0.0010	1.1009±0.0013	59
P/L 1	3.0805±0.0016	1.1359±0.0024	59

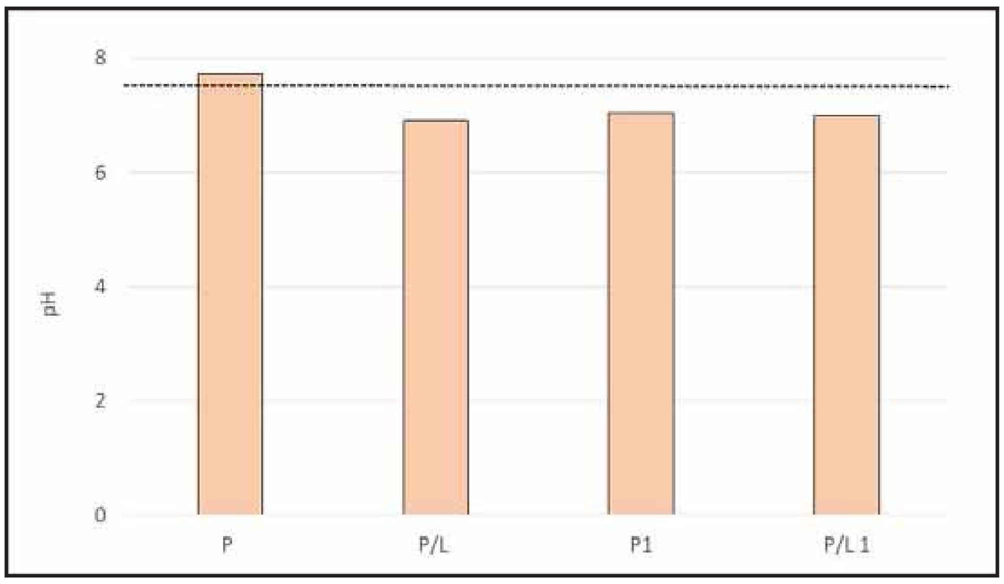


Fig. 7. pH of the prepared aggregates

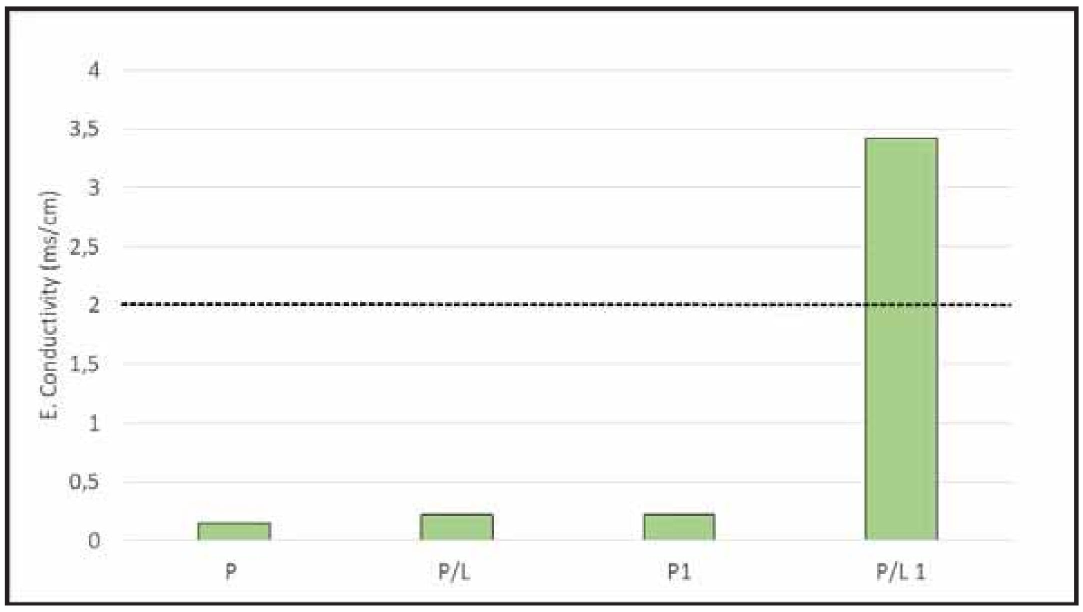


Fig. 8. Electrical conductivity of the prepared aggregates

4. Conclusions

In this preliminary study the feasibility to use the volcanic inert scraps in the manufacturing of geo-polymers and lightweight aggregates was demonstrated. The research proposed to avoid the landfill disposal of both the volcanic inert finer fraction and the spent coffee grounds used as pore-forming agent. On the basis of the findings, the following specific conclusions can be drawn.

Geo-polymers:

Volcanic minerals are suitable to obtain geo-polymeric materials; their presence does not hinder geo-polymerization process. pH remains constant with values typical for metakaolin geo-polymers. Conductivity shows different behavior depending on the presence of pumice or lapillus. Pumice maintains low values while lapillus leads to higher values of conductivity. This can be related to the chemical composition of lapillus richer in Ca, Mg and Na, but also to the more porous structure of lapillus-based geo-polymers. Further, compressive strength is particularly high for geo-polymers containing lapillus; in particular, this one confirms its stability both chemically and mechanically.

This research will help to support the choice of matter recycling as viable alternative and reduce CO_2 emissions in building manufacturing.

LWAs:

All compositions tested resulted in lightweight aggregates according to the standard UNI-EN. Furthermore, these aggregates have water absorption values and total porosity of the same order as commercial products like Arlita Leca L used in gardening, horticulture and roof insulation applications. Besides, they present adequate pH and E.C. values to be used as growth substrates in agronomic applications.

The complete replacement of natural clay minerals with inert volcanic scraps and the use of post-consumer residue (SCGs) represent an interesting alternative to manufacture lightweight aggregates for agronomic purposes (draining and fertilizer materials), using low sintering temperature with less environmental impact and economic savings.

Acknowledgments

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AQUEOUS EXTRACTS AND RESIDUAL BIOMASS USE IN SUSTAINABLE AGRICULTURE: A CIRCULAR ECONOMY MODEL

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Abstract

The circular economy is based on sustainable production and consumption. In terms of circular economy, sustainable agriculture is achieved through the effective use of internal resources to self-produce and use, without waste production, green preparations for the fertilization and protection of crops. In this context, the project of a certified organic farm aims to cultivate medicinal plants to self-produce aqueous extracts of thyme and tansy, for use in crop protection, and reuse residues for composting and mulching. Regarding the environmental and economic impact, a virtuous process of cultivation and defense of agricultural crops was carried out (three-year rotation of zucchini-cabbage-chicory), to respond to market demand and to implement safety and health protection policies for farm workers and consumers. In a preliminary germination test, a stimulating effect was observed on *Vicia faba* seeds treated with thyme extract in which the greater elongation of the primary roots, relative to the control, was statistically significant. The effects of the extracts on the crops (weight and chlorophyll content) have always been significant. In particular, the chlorophyll content of chicory is highly significant for the remaining parameters measured for all horticultural crops in the field trial.

Key words: aqueous extracts, circular economy, composting, mulching, natural farming

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1. Introduction

In December 2015 the European Commission established an Action Plan for the circular economy, defining an economic development model in which resources must be exploited and waste used as raw material to create new production cycles and to protect the environment and reduce greenhouse gas emissions (GHG) (EC, 2015; Kirschenmann, 2010). The action plan also includes the EU Fertilizers Regulation (EC, 2018) which encourages production and trade of sustainable fertilizers (EC, 2009), including compost, produced by recycling organic waste, which can be used in agriculture (EC, 2016; Turcanu, 2018).

Agriculture, being a primary production sector, plays a fundamental role in terms of circular economy. Therefore, circular agriculture represents an innovative agricultural system in which everything is reused and regenerated, becoming a valuable resource. Savings is one of the main advantages of the circular

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economy in agriculture, since the reuse of waste and the self-production of fertilizers eliminates the problem of waste disposal at the end of the cycle, allowing a significant reduction in management costs and reducing the environmental impact caused by the use of synthetic products derived from non-renewable fossil sources.

In agriculture, too, the circular economy is becoming an increasingly relevant concept, as an important component of the transition to sustainable development. In fact, it is proposed to reduce the production of waste and residues deriving from productive activities (agroforestry, fishing, animal husbandry, processing of agricultural products, trade, agricultural services and consumption of products) (Albiach et al., 2000; Zaccardelli et al., 2007) as much as possible in order to develop an economic system based on recycling and sustainable agriculture.

Natural farming is an innovative method of cultivation that is suitable for the circular economy (Benyus, 2002), especially for horticultural crops, due to the self-production of the main technical means, such as compost and plant extracts, in order to improve productivity and the self-defense of the cultivation system.

Disposal of plant crop residues is an issue, especially in areas where there are many greenhouses with green biomass left outdoors to dry and decompose, instead of significantly reducing biomass residues and treating them through a recycling system (De Corato et al., 2018; Esparza et al., 2020). Since the chemical composition of biomass determines many of its properties, special emphasis should be placed on organic crop products and wastes that are free of synthetic substances present in plant protection products.

Within a certified organic farm, it is possible to apply the principles of the circular economy to self-produce and use effective plant preparations for crop fertilization and protection, using waste biomass for mulching and compost production. Chemical products are not used in natural agriculture, the treatments applied involve only self-produced technical means, such as compost, used as mulching material to create a layer of permanent homogenous soil, or aqueous plants extracts used as basic substances to support crop protection (Dayan et al., 2009; Gurjar et al., 2012). Plant extracts and substances that strengthen the plant's natural defenses (plant reinforcements), used in crop protection, could be included in the list of basic agricultural aid substances (Beni, 2020; Marchand, 2017).

Soil mulching with various types of bedding is done to prevent weed growth, protect soil from erosion, maintain soil moisture and prevent surface crusting, reduce compaction, safeguard structure, and increase soil temperature. Composting also makes it possible to transform the starting substrate into a stable product, similar to humus, used in soil fertilization (Sayara et al., 2020; Sleutel et al., 2003; Sleutel et al., 2006). The work being presented here is the result of a project for the construction of a sustainable farm based on a circular economy management principle. The experimentation started with preliminary tests and field tests carried out at the CREA experimental fields located in Tor Mancina (Beni et al., 2020), and then continued at an organic farm located in Poggio Mirteto, both near Rome.

In this project, aqueous extracts from self-grown medicinal plants were investigated as bio-stimulants and adjuvants in agricultural crop protection. Plant extracts were chosen because, being a mixture of compounds, they provide greater activity than the single active ingredient, thus being more effective and not presenting particular toxicity to workers and the environment. This phenomenon, known a synergism (or synergy) (Hummelbrunner and Isman, 2001; Singh et al., 2009), induces better and longer lasting effects (Chockalingam et al., 1990) than a simple additive effect.

In a recent study, seaweed extracts improved abiotic stress tolerance of horticultural crops and acted as protective and growth-promoting factors, as well as antibacterial agents. The mode of action was related to shoot growth, root growth, fruit set and quality (Michalak et al., 2020). A two-year pot experiment was conducted to evaluate the effect of NPK fertilizer, garlic extract and their combinations on growth, flowering and chemical constituents of *Hedychium* plants. The fertilization of *Hedychium* plants with a NPK fertilizer (19:19:19) at 4 g pot^{-1} and spraying with a 50% garlic extract is considered the best treatment, also economical, used to enhance growth, flowering and improve the nutritional status of the plant (Attia et al., 2020).

Two experiments were conducted in Egypt to define the effect of neem, liquorice, turmeric, pomegranate and thyme extracts to control mechanical damage, increasing productivity and storability of potato plants. Foliar spraying with pomegranate peels or liquorice extracts (5%) significantly increased growth parameters, total tuber and marketable yields and decreased mechanical damage of potato. Application of pomegranate or thyme extracts significantly reduced the percentage of weight loss and decay, and increased starch and dry matter content compared to control and other treatments during storage at 4°C. This study recommends the use foliar applications with thyme extracts to increase storability and reduce weight loss, at 15-day intervals in spring (Ezzat et al., 2016).

In a study conducted on cucumber plants (*Cucumis sativus*, var. *Korinda*), the effects of *Artemisia absinthium* and *Tanacetum vulgare* extracts, against *Thrips tabaci*, were compared to a corresponding commercial product containing the same extracts, using a water treatment as a control (Helm, 2015). Histological characterization was carried out by checking the thickness of the leaf epidermis. Plants treated with the three treatments showed thickening of the cell walls of the epidermis compared to the control plants. The pectin colour of the leaves treated with the products was greater than those treated with water.

The manuscript presents the first results of innovative farms with a closed-cycle production, entirely inspired by the circular economy model. The farms self-produce most of the technical inputs used for growing vegetables and herbs. All fertilizers, substrates, crop-protection products, basic substances, phyto-stimulants and mulches used in the production cycle are of natural origin, obtained from primary production biodegradable waste. Even the seeds and cuttings for the reproduction and propagation of vegetables and aromatic plants, used as beneficial companion plants, are self-produced by the farms.

In previous work, 12 natural aqueous extracts (garlic, burdock, horsetail, hypericum, lavender, lantana, pomegranate, mint, oregano, sage, tansy and thyme) were initially tested (Casorri et al., 2014) and subsequently only the extracts of garlic, thyme, and tansy, were tested since they proved to be the most effective in controlling pests and diseases of agricultural plants (Beni et al., 2018a; Beni et al., 2018b; Beni et al., 2020; Casorri et al., 2014; Masciarelli et al., 2019; Rinaldi et al., 2019). The tests were carried out in the open field at CREA experimental farms, on zucchini (*Cucurbita pepo L.*) cv. Augusto (Romanesco type) to verify the effectiveness of 1% and 2% w / v aqueous extracts, as insecticides and as fungicides against *Podosphaera xanthii* (Casorri et al., 2014). The results obtained showed that all the zucchini plants treated with extracts of garlic, thyme, lavender, sage, mint, oregano and tansy showed greater resistance to parasitic attacks and bio stimulating effects compared to untreated plants (Casorri et al., 2014).

Indeed, treated plants, particularly with thyme, garlic and tansy extracts, were characterized by a greater vegetative vigor, a better floral induction, a higher chlorophyll content and a greater number of fertile flowers, compared to untreated plants. Furthermore, zucchini production per plant was statistically higher than controls (Beni et al., 2018b; Beni et al., 2020; Casorri et al., 2014; Masciarelli et al., 2019).

This work illustrates the experimentation, which is still in progress at the organic farm located in Poggio Mirteto, and concerns the protection of plants and their bio-stimulant effect by means of aqueous extracts of thyme and tansy, self-produced from officinal plants grown on the same farm and the reuse of residual biomass deriving from the cultivation and processing of all agricultural products of the farm, typical of the Mediterranean area for size and productive orientation. The phyto-stimulating properties of thyme and tansy extracts are able to activate a protective effect in the treated plants in response to adverse conditions (oxidative stress), which depends on the chemical composition of the phyto-complexes within the broad spectrum of molecules in solution in the extracts (Posmyk and Szafranska, 2016). Tansy (*Tanacetum vulgare*) has strong insect repellent properties. Through biological assays, the greater repellent efficacy was associated with the presence of 1,8-cineole, bornyl acetate, p-cymene, γ-terpinene and camphor, while the insecticidal properties to β-thujone. B-thujone (tanacetone) is present as a major component in the b-dextrorotatory form. It is a terpenoid containing a ketone group having two stereoisomeric forms known as (+) - 3-thujone or α-thujone and (-) - 3-thujone or β-thujone. It has a menthol smell and has an insecticidal effect (ants, aphids, lepidoptera, agrotids, moths and borer) and pesticide. Thanks to these properties it is used to disinfect gardens and vegetable gardens (Brewer and Ball, 1981; Dancewicz and Gabryś, 2008; Dancewicz et al., 2011; Kwiecień et al., 2020).

Thymol and carvacrol are the main constituents of thyme (*Thymus vulgaris*), responsible for effectiveness. (Saqvic et al., 2007). Thyme extract, due to its antiseptic, antibacterial, antifungal and antioxidant properties, can be used as a fungicide in agriculture, but it also has a good nematicide activity (Zaccardelli et al. 2007). Thymol is a monoterpenes' phenol characteristic of plants of the genus *Thymus*, contained throughout the plant and important for its antibacterial properties and characteristic odour. It is a particularly effective fungicide. Carvacrol (cymo-phenol) is also a monoterpenes' phenol present in *Thymus* and *Oregano*. Thymol and carvacrol act through a synergistic effect. The antioxidant properties of thyme are instead due to the content of polyunsaturated flavonoids (Kulisic et al., 2005; Szilvássy et al., 2013).

This work aims to show the possibility of creating an independent organic farm that can manage the production, protection, and control of crops in a sustainable regime and protect the environment and the health of agricultural workers and consumers and in the perspective of the principles of the circular economy.

2. Materials and methods

2.1 Preparation of the aqueous extracts and their chemical characterization

The extracts of tansy (*Tanacetum vulgare L.* subsp. *Vulgare*) and thyme (*Thymus vulgaris* var. *Verticillata* Willk) at 1% w/v were prepared in distilled water at a temperature of 25° C using thyme leaf powder and tansy flowering tops, dried in a thermostatic chamber at 40° C. Solute percentages were chosen based on guidelines provided by the producers' association in order to produce useful substances in organic and natural agriculture. The extracts, filtered after 48 h on filter paper, were either directly used or stored at + 4 ° C for 6-7 days. For crops treatments, the extracts were used without dilution, as indicated by the association of natural and organic producers (Nashwa and Abo-Elyousr, 2012).

The extracts were subjected to chemical analysis, phytotoxicity tests and field tests. (Beni et al., 2020).

2.2. Phytotoxicity test

In this experimentation, laboratory tests were performed to evaluate the potential toxicity of the aqueous extracts prepared with thyme and tansy produced within the organic farm. To perform phytotoxicity tests, fava bean (*Vicia faba* var. *minor* Beck) seeds were allowed to germinate in a quartz sandy soil (Sturchio et al., 2006) treated with thyme or tansy extracts. To perform the tests, 25 fava bean seeds were placed on 250 g of quartz sand in each of 9 aluminium boxes. Three boxes were treated with 100 mL of thyme extract, three boxes were treated with 100 mL of tansy extract, and three control boxes only with deionized water (100 mL) to wet seeds. Each box, sealed with Parafilm, was incubated for 5 days at 20±1 °C to allow seed germination.

The effects of both the aqueous extracts on seed germination were examined. In particular, the primary root length reduction (PRL) test was used to evaluate the phytotoxic effects through growth inhibition. After 5 days, 100% of the seeds had been germinated and each of the 75 primary roots was measured with a calliper, placing each root on a flat surface after washing.

2.3. Field trial

An open field trial was conducted on a certified organic farm located in Poggio Mirteto, about 50 km north of Rome. The farm began converting a portion of the vegetable garden to natural farming in 2016. Natural farming aims at the self-reinforcement of undisturbed soil fertility. Tillage is not carried out, except for the preparation of the cultivation beds at the beginning of the conversion, prepared by taking the topsoil from permanent walkways. None of the chemicals allowed in organic farming were used. The only application made concerns self-produced technical means, such as green compost, integrated into the mulch in order to accelerate the creation of a permanent homogenous topsoil layer, or plant aqueous extracts used as basic substances to support crop defense (Beni et al., 2018b; Cappello, 2019; Fiebrig et al., 2020; Fini et al., 2016; Hazelip, 2014; Mancin, 2012; Marchand, 2017; Pinamonti, 1998; Rezendes et al., 2020; Rinaldi et al., 2019; Shyam et al, 2019).

By means of analyses conducted according to official methods (MiPAAF, 2000), the soil was characterized as a clayey-silty texture with a high content of total organic carbon (4.7%), a sub-alkaline pH (7.4) and a significant cation exchange activity (35.86 meq 100 g^{-1}).

The soil was only tilled prior to conversion, to shape raised beds approximately 0.4 m high, 1 m wide and 5 m long. On the beds, mulching is carried out with self-produced green compost and renewed every 6 months, before each productive cycle. This operation has the dual purpose of containing the germination and growth of wild plants and improving soil fertility by creating a homogenous top-soil layer. The compost is self-produced by the farm, using the biodegradable waste from the pruning of olive and fruit trees and vegetable residues. The compost is turned over and moistened weekly for the first 21 days during the stabilization phase, then it is left to mature for six months to be used as mulch. In this last phase, passive ventilation is carried out by placing perforated pipes inside the pile of biomass being oxidized. The characteristics of the compost produced in the period 2018-2020 are described in Table 1.

Table 1. Chemical composition of the self-produced compost

Parameter	*Measurement unit*	*Value*
Moisture	%	35-42
pH	-	6.5-8.2
TOC	% d.m.	24-31
Total N	% d.m.	1.7-2.3
C/N	-	13-16
P	% d.m.	1.1-1.8
K	% d.m.	2.2-3.5
Cu	mg kg^{-1}	91-112
Zn	mg kg^{-1}	254-311
Germination rate (dilution 30%)	%	73-88
Salmonella	MPN	Absent
Escherichia coli	UFC g^{-1}	< 1.000

Evaluation of the effects of the extracts was carried out in the open field on zucchini-cabbage-chicory plants in a three-year rotation. On each bed, the following plants were respectively transplanted: 6 courgette plants (*Cucurbita pepo L.*) cv. Augustus (Romanesco type) on 9 April, 2018; 40 cabbage plants (*Brassica oleracea L.*) cv. Savoy King on April 16, 2019; and 50 chicory plants (*Cichorium intybus L.*) cv. Catalonia on May 7, 2020. Nine beds were divided into three blocks, and the plants on one bed per block were sprayed weekly with thyme or tansy extracts at a concentration of 10g L^{-1}. As a control, a bed per block was used whose plants were sprayed with water and compared with those treated with thyme and tansy extracts. Three zucchini plants, nine cabbage and chicory plants were randomly selected and marked to detect yield. Zucchini were harvested at 14 different times, from the end of May to the end of July, and the harvest data were summarized.

2.4. SPAD measurements

To evaluate the vegetative state of each plant, in vivo measurements of chlorophyll content was carried out with the SPAD 5200 portable fluorimeter (Konica Minolta Business Solution Italia Spa, Milan, Italy) on the leaves of the three species. Measurements were made for courgette in the middle of the harvest period and before harvest for cabbage and chicory, with three replicates per plant on each cultivation bed.

2.5. Statistical analysis

The experimental data of plant weight (g $plant^{-1}$), SPAD units, and phytotoxicity tests (PRL test), were previously analyzed by graphical analysis (box plot) and descriptive statistics to estimate the variability and determine possible outliers. Homoscedasticity of the data was checked using Levene's test. Two ways ANOVA was performed to check the effect of two extracts on the vegetable plants on the field and on bean seeds, compared to the untreated control. Comparisons between treatments means were done when test F of ANOVA was significant (α level=0,05) using Tukey's HSD test.

3. Results and discussion

The results of the phytotoxicity test and the three-year rotation field test are presented in Table 2 and Table 3.

3.1. Phytotoxicity test

The Primary root length (PRL) test was significantly affected by the effect of the extracts, as shown by the ANOVA F test (Table 2). No repressive induction on primary root growth was detected compared to the control, thus excluding any phytotoxic activity. On the contrary, a stimulation effect was observed on seeds treated with thyme extract in which the greater elongation of the primary roots, compared to the control, was statistically significant.

3.2. Yield and chlorophyll content of crops in three-year rotation

The two-way ANOVA has never detected any significance for the effects regarding the blocks of beds, while the effects of the extracts on vegetable weight and chlorophyll content (SPAD units) in all horticultural crops were always significant. In particular, the ANOVA test F, shown in table 3, confirms that the effects of the extracts were significant for the SPAD units of chicory (*p value* <0.05) and remarkably significant (*p value* <0.01) for the remaining parameters measured for all horticultural crops in the field trial.

The data in Table 3 shows the effects of the extracts on the yield expressed as weight of the edible portion per plant and on chlorophyll content of crops. In particular, for zucchini, the thyme extract significantly increased the weight of the vegetable by 22.44% compared to the control; also, the tansy extract increased the vegetable weight by 8.04% compared to the control but without statistical significance. Regarding the SPAD units, treatments with tansy and thyme extracts both significantly increased the values of this parameter by 21.9% and 25.17%, respectively. In cabbage, both extracts, highly significantly (test F, *p value* <0.01) and similarly, increased the weight of the vegetables and the SPAD units, compared to the control.

Table 2. F ANOVA and PRL test (mm) in fava beans treated with tansy and thyme Extracts (mean and standard deviation sd)

F ANOVA[(a)]	***7.652 (p value < 0.01)***		
Extracts	***N. of seeds***	***PRL (mm)***	
		Mean	***sd***
Control	75	89.89 a	10.27
Tansy	75	88.09 a	11.30
Thyme	75	94.55 b	9.79

Means marked with different letters are significant on Tukey's HSD test (p-value <0.05);
[a)]Degree or freedom 2;216 (extracts: error);

Table 3. F test ANOVA, Vegetable weight and SPAD units in plants treated with thyme and tansy extracts (mean and standard deviation sd)

Vegetable Crops (year)		***Vegetable weight (g plant-1)***		***SPAD Units***	
Zucchini (2018)	***F ANOVA (a)***	***7.357 *****		***18.33 *****	
		mean	***Sd***	***mean***	***Sd***
	Control	5215.89 a	768.08	33.34 a	2,73
	Tansy	5635.22 ab	529,43	40.64 b	2.53
	Thyme	6386.33 b	661.89	41.73 b	4.18
Savoy cabbage (2019)	***F ANOVA (a)***	8.177 **		13.417 **	
		mean	*Sd*	*mean*	*Sd*
	Control	1329.22 a	87.87	25.67 a	4.22
	Tansy	1520.44 b	166.19	36.29 b	5.61
	Thyme	1593.89 b	130.85	36.59 b	5.14
Chicory (2020)	***F ANOVA (a)***	8.129 **		5.297 *	
		mean	*Sd*	*mean*	*Sd*
	Control	486.22 a	88.27	41.43 a	5.29
	Tansy	651.78 b	74.56	50.29 b	5.07
	Thyme	566.44 ab	86.56	44.21 ab	5.86

***(p value < 0.01); * (p value < 0.05), The means marked with separate letters, in the columns concerning the same crop, were significant in Tukey's HSD test (p value <0.05), (a) Degree or freedom 2;18 (extracts: error)*

As a mean of two treatments, weight gain was 17.15% (+227.95 g) and in SPAD units 41.96% (+10.77 units), compared to control. In chicory, tansy extract significantly increased the yield of the edible portion by 34.05%, compared to the control. Thyme extract also allowed yields that were 16.50% higher than the control, although not statistically significant. Similarly, the SPAD units in chicory were significantly increased by 21.39% from the tansy extract compared to the control, while the 6.71% increase induced by the thyme extract, compared to the control, was not statistically significant.

4. Conclusions

The concept of circular economy takes inspiration from the natural cycle and is perfectly applicable to the agricultural sector. Agricultural biomass can be used for the autonomous production of plant extracts useful for crop defence, and their waste exploited in mulching and fertilization operations. Plant extracts have proved to be effective auxiliary technical means in the defence of crops. Furthermore, the extracts showed no toxic effects; on the contrary, they were antioxidants and bio stimulants, effective in increasing the growth and production of vegetables. The treated plants had, compared to the untreated, a greater vegetative vigour and a greater production of flowers and fruits.

The gradual replacement of conventional plant protection products and fertilizers with natural preparations, such as plant extracts, will provide significant benefits in protecting human health and reducing occupational and environmental risks, via pest management with low pesticide intake. This virtuous process of agricultural defence is more advantageous in terms of circular economy and provides for a more efficient use of resources that responds to the needs of the market, environmental safety, and health protection policies for consumers and agricultural workers.

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COMPARISON BETWEEN COFFEE AND COMMON LIGNOCELLULOSIC BIOMASS FOR ENERGETIC POTENTIAL PREDICTION

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Abstract

Energy production from renewable and waste materials is an attractive alternative to conventional production chains that involve agricultural products. Residual biomass from cultivars and coffee production chain, despite their widespread availability, aren't enough considered in energy models and economic development. In addition to lignocellulosic biomass, coffee can be considered as a new material usable in such processes. ICO (International Coffee Organization) data showed that the Spent Coffee Grounds (SCG) production worldwide is about 6 million of tons per year. In the work presented, calorific value, ash content, and elemental analysis of lignocellulosic biomass and SCG pellets, were firstly examined. The aim was to compare SCG with conventional lignocellulosic biomass already used in thermal production. Compositional and energetic analysis permit to fix linear models for biomass energetic yield prediction. Models that relate the higher heating value (HHV) to the compositional analysis mostly date to the late 19th century. Estimation of HHV from the elemental composition of fuel is one of the basic steps in performance modelling and calculation for thermal systems. The possibility to perform statistical analysis on data collected in the same laboratory gave the opportunity to reliably compare conventional and unconventional biomass. The linear regression model fitted on the whole dataset had an R Squared of 0.85 showing a good HHV prediction from elemental analysis. Coffee appeared as a feedstock with peculiar characteristics that differentiate it from the others, while herbaceous and arboreal biomass mostly differentiated for ash and moisture content.

SCG showed an HHV higher than any other woody and herbaceous plant, manifesting a great potential from an energetic point of view. According to the concept of circular economy, coffee companies, in their waste, have already a valid resource usable in a heat generator for the roasting process.

Key words: biomass, modelling, spent coffee grounds (SCG), ultimate analysis

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1. Introduction

Large amounts of agricultural and forestry residues, usually treated as waste, can be considered as a significant resource for energy production through biological or thermo-chemical processes (Bianchini et al., 2021; Carnevale et al., 2020; Paris et al., 2019a; Schmitt et al., 2019; Sun et al., 2018). To date, processes and models for the exploitation of lignocellosic biomass are mainly based on forest resources (Tomassetti et al., 2019; Torre et al., 2019). Despite the considerable volumes produced, residual biomasses from agricultural crops are rarely considered in energy models and economic development. Alternative energy sources are increasing their importance both to meet the energy

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growing demand and to reduce the environmental impact. Given the high volumes produced every year, soluble coffee residues represent an important unexplored resource in the agro-industrial sector. Coffee has one of the most developed markets in the world and together with tea, it is among the most consumed beverages (Park et al., 2019). Its annual worldwide generation reach the 6 million tons (Mussatto et al., 2011). The organic molecules present in coffee suggest that the recovery of such resource can be economically advantageous, leading to the synthesis of valuable compounds. (Kibret et al., 2021; Kondamudi et al., 2008; Kua et al., 2016; Liu et al., 2017; Murthy and Madhava Naidu, 2012; Mussatto et al., 2018). Studies regarding the potential thermal exploitation of spent coffee grounds (SCG) are increasing and the reason of such interest in coffee waste is explained by its big market volume. ICO (international Coffee Organization) data showed that the apparent consumption of coffee in Italy between 2004 and 2016 oscillates from 5.46 to 6 million of 60 kg green bean bags (Sette, 2017).

The large amount of waste production in the coffee market unavoidably leads to questioning on the possible utilization of such waste inside a circular economy model. Combustion is one of the thermal production processes more rooted and used in common living, especially through the domestic fireplace and stoves. The feasibility of SCG thermal valorization has to be discussed both from the logistic and energetic point of view (Volpi et al., 2019). The possibility to use a new material like coffee in established thermal conversion methods was already investigated in previous works (Colantoni et al., 2021; 2020). Biomass fuels are considered a renewable resource both for their continuous production and because they do not affect the overall balance of CO_2 in the atmosphere.

Knowing the physicochemical properties of biomass is essential for its use in power plants. These raw materials are experimentally characterized by analyzing the elemental composition, energy efficiency, and fusibility of the ashes (Pari et al., 2018). Such analyzes are regulated by standards to ensure the quality and comparability of the measurement results. The calorific value of biomass is a fundamental parameter for the exploitation of this type of fuel in power plants. The higher calorific value (HHV) consists of the amount of heat produced by the complete combustion of a unit quantity (by mass or volume) of fuel under certain conditions, when the reaction pressure is kept constant. The lower calorific value (LHV) is obtained when the energy used for the evaporation of the water formed during combustion is subtracted from the total energy produced. Numerous models have been published to relate the energy produced by the fuel to the elemental composition of the fuel itself. (Friedl et al., 2005). For these reasons, the calorific value of such wastes is regarded as the most significant parameter that defines the fuel quality. The estimation of the calorific value based on the chemical composition of biomass has also been in great demand when reliable analysis results are present.

Macromolecular ingredients such as hemicellulose, cellulose, and lignin account for most of the organic part of the biomass while some others include starch, proteins, triglycerides, lipids, etc. Accordingly, some kinds of biomass, particularly woody ones, are generally defined as lignocellulosic. On the other hand, although these macromolecular components are consisted mostly of carbon, hydrogen, and oxygen, their molecular configurations and structures are highly different (Ozyuguran et al., 2018).

Many correlations for the estimation of HHV from elemental composition are available in literature, the most important have been presented in Channiwala and Parikh (2002), and most of these relations have been derived for coals. Furthermore, the majority of these correlations, when referred to lignocellulosic biomass, use mixed datasets with data provided from different studies, obtained with different instruments and sometimes with different methods. To carry out the analyzes in the same laboratory permits to minimize the data variability coming methods, instruments and operators. For these reasons, the present work is marked with the intention to create a homogeneous dataset to set up the HHV modeling from compositional analysis of different kinds of biomass.

2. Materials and methods

2.1. Biomass description

The biomass coming from different projects and relative works, were collected for more than a year, starting from October 2019. The modeling analysis has been carried out on 41 samples composed of different mixtures of lignocellulosic biomass. The complete biomass description is provided in Table 1.

2.2. Ultimate and proximate analysis

Ultimate and proximate analysis was carried out adopting always the same procedure following European standards for biomass characterization. The biomass humidity was measured through the Memmert UFP800 drying oven at a temperature of 105 ± 2°C for 24 hours, according to ISO 18134-2 (2017). For characterization, the dried sample was grinded first with the Retsch SM 100 cutting mill for a preliminary size reduction and thereafter through the Retsch ZM 200 rotor mill.

Ash content was measured by a Lenton EF11/8B muffle furnace according to ISO 18122 (2015). The higher heating value (HHV) was determined by the Paar 6400 isoperibol calorimeter following the ISO 18125 (2017), while the lower heating value (LHV) was calculated from the higher heating value, according to ISO 18125 (2017).

Table 1. Biomass used for experimental and modeling analysis

Biomass	***Group***	***Appearance***	***References***	***Notes***
Grapevine	Fruit Cultivar Tree	Chipwood	Proto et al. (2021)	*Vitis spp*. Harvested in Calabria, Southern Italy
Olive	Fruit Cultivar Tree	Chipwood	Proto et al. (2021)	*Olea spp*. Harvested in Calabria Southern Italy
Citrus	Fruit Cultivar Tree	Chipwood	Proto et al. (2021)	*Citrus spp*. Harvested in Calabria Southern Italy
Cultivars mix	Fruit Cultivar Tree	Pellet	Vincenti et al. (2020)	Mixed pellet of *Citrus*, *Olea*, and Kiwi (*Actinidia spp*) harvested in Calabria, southern Italy
Wheat straw	Straw Herbal	Chipwood	Paris et al. (2019b)	*Triticum aestuvum L*. produced by the CREA of Monterotondo
Rice straw	Straw Herbal	Chipwood	Paris et al. (2019b)	*Oryza sativa L*. imported from different areas of Pakistan (Punjab, Azad Jammu and Kashmir (AJK), and Sindh)
Hemp	Hemp Herbal	Chipwood	Not published	*Cannabis spp*. Produced by the CREA of Monterotondo
Forest mix	Forest Tree	Pellet	Vincenti et al. (2020)	Mixed pellet of fir (*Abies spp*), beech (*Fagus sylvatica*) and chestnut (*Castanea sativa*)
Coffee	SCG	Pellet	Colantoni et al. (2020; 2021)	*Coffea spp*. Mixed pellet obtained with different sawdust percentages (0, 15, 25, 33, 66)

The elemental composition, carbon content (C), hydrogen content (H), and nitrogen content (N) was measured with the elemental analyzer Costech ECS 4010 CHNS-O according to ISO 16948 (2015).

2.3. Statistical analysis

The statistical analysis was entirely conducted in R ver. 3.6.1. Different statistical tests and analysis resulted useful for the data comprehension. Since the biomass' description was one of the goals of this study, differences between species were tested through a One-Way ANOVA at the 0.05 significance level, permitting to evaluate the importance of the biomass factor on energetic and compositional parameters. The individuation of such differences is subsequently obtained with the post hoc Tukey-HSD test, able to compare groups means and to define weather the variables assumed significant differences according to the plant species. Shapiro-Wilk and F tests were performed to evaluate both normality and homoscedasticity of biomass characterization variables. Since many variables didn't show a Gaussian trend, the Friedman test and the Conover test were performed to understand the difference between biomass. The multivariate data analysis was conducted by Principal Component Analysis (PCA) to evaluate the relationships between biomass properties. The cluster analysis was performed by the Ward technique, whose aim is to achieve a hierarchical classification by minimizing the variance of the variables within each group. At each stage, the groups that produce the smallest increase in the total variance within the groups are merged (Ward, 1963).

Since the characterization variables are neither normal nor homoscedastic, the quantile regression (QR) has been used to build linear models able to predict HHV from C, H, and N. This method results more accurate when the basic requirements for applying ordinary least squares (OLS) are not met, particularly in the presence of outlier values. Quantile regression is able to provide a much broader analysis of the relationships between variables than the OLS model. Over the years, QR has been used as an extension of the linear regression model and it allows to do the analogue of what linear regression does for the mean, on quantiles. By exploiting the estimated parameters, it is possible to consider the quantile value of the response variable, depending on a set of regressors. This allows to appreciate the behavior of the response variable not only in average but also in its entire distribution. By varying the quantile of the regression between zero and one (τ) it is possible to obtain the entire conditional distribution. To evaluate the forecast quality, the root means square error (RMSE), mean absolute error (MAE) and mean bias error (MBE), were calculated. The MBE gives information regarding the average forecast error representing the systematic error of a forecast model, MAE gives the forecast errors average magnitude, while with RMSE more weight is attributed to the largest errors (Kato, 2016).

3. Results and discussion

3.1. Proximate and Ultimate Analysis

From the proximate and ultimate analysis (Fig. 1), SCG resulted a biomass with peculiar characteristics, both from a compositional and an energetic point of view. The samples listed in Table 1 were grouped in three branches depending on the physical structure of the biomass: Coffee, Herbal and Tree (Fig. 1). Through the Friedman test applied to compositional variables, real differences are pointed out. It's clear that SCG has more C and N percentages

(Fig. 1a-b) than herbaceous and arboreal biomass at the expense of H, which shows a very low content for SCG (Fig. 1c). Many other studies, concerning both biomass and hydrocarbons (Demirbas et al., 2018; Ozyuguran et al., 2018), relate the compositional analysis to the HHV. For biomass, in general, it is overt that C is strictly positively related to HHV. In this case, coffee is a very surprising material, inasmuch its HHV is significantly higher than any other biomass taken into account (Fig. 1d). Proximate analysis concerning humidity and ash reveals coffee as a biomass with a higher content in water and normal content of ash.

Regarding the elevated humidity tenor (Fig. 1e), it is due to the nature of SCG which derives from a process where coffee is crossed by water. In this case, processes related to transportation, stock and drying are fundamental (Schmidt Rivera et al., 2020). The other two kinds of biomass, arboreal and herbal, usually behave in a similar way except for C, HHV, and ash. Herbaceous biomass has the worst energetic characteristics with lower HHV and C content, and higher ash production during combustion (Fig. 1f). Such data indicate low potential in thermochemical conversion processes.

3.2. PCA analysis

Some of the trends described above can be more formally elucidated through the application of multivariate statistical techniques. Other studies already tried to classify different lignocellulosic biomass through a multivariate approach (Jenkins et al., 1998). Fig. 2 gives PCA results using the ultimate and proximate analysis for the 41 observations in the dataset. Differences between the four main classes have been highlighted in the figures: straw, coffee, wood pellet, and wood chip. Fig. 2 is a plot of the first principal component PC1 respect to the the second principal component PC2.

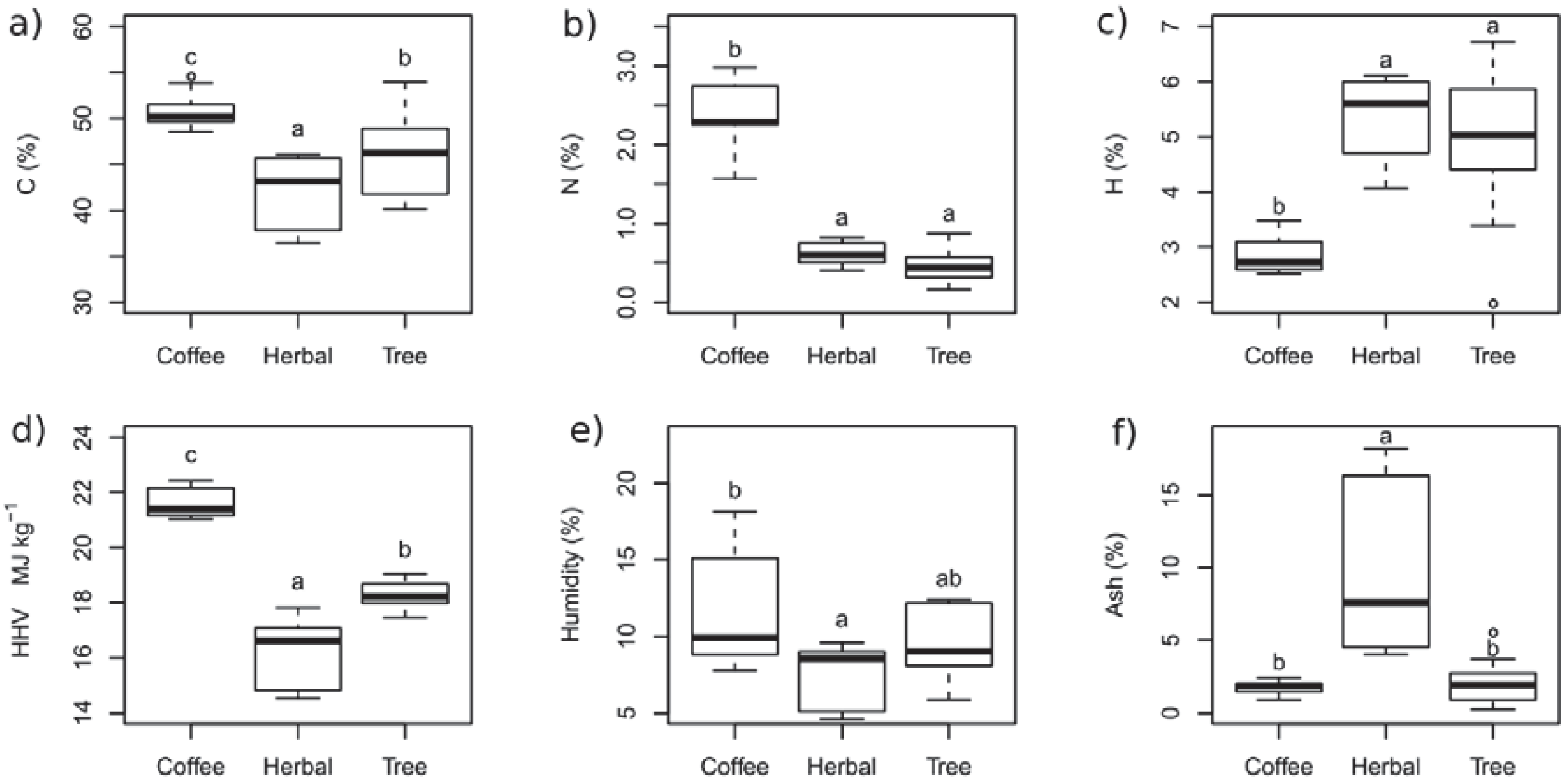

Fig. 1. Boxplots of ultimate and proximate analysis parameters for Coffee, Herbal and Tree biomass. Carbon content (a), Nitrogen content (b), Hydrogen content (c), Higher Heating Value (d), Humidity (e) and Ash content (f). The boxes represent the minimum (Q1 - 1.5*Interquantile Range), 25th percentile (Q1), 50th percentile (Q2), 75th percentile (Q3) and maximum (Q3 + 1.5 Interquantile Range). Groups with different letter are significantly different by using post hoc Tukey-HSD test ($p<0.05$)

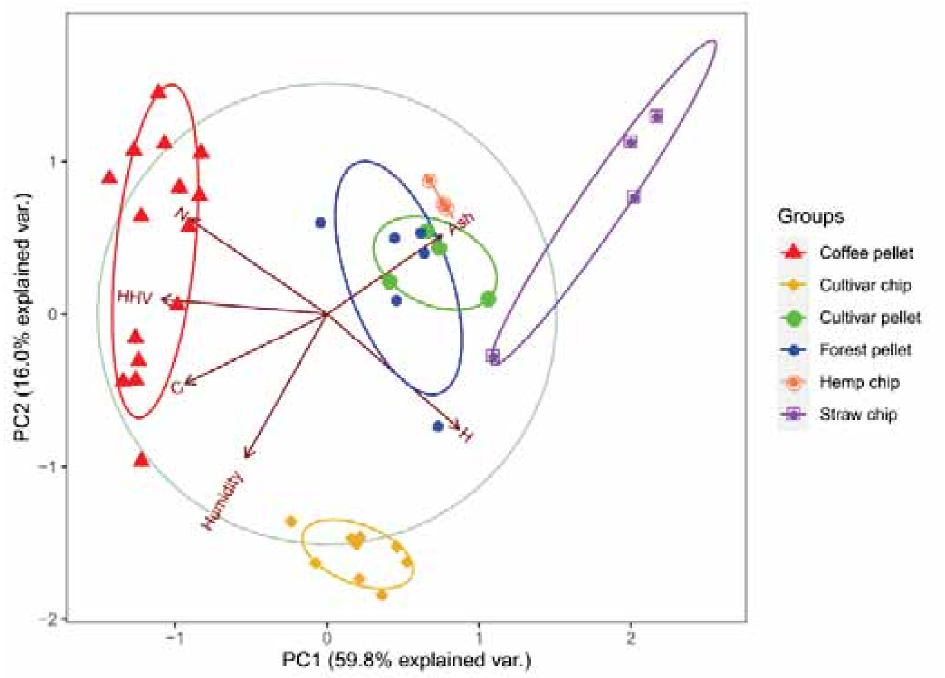

Fig. 2. Principal Component Analysis biplot obtained with the parameters obtained from ultimate analysis and proximate analysis

These two components explain the 75.8% of the total variance in the data. PC1 has a strong negative correlation with HHV, C, and N, while a positive correlation is shown for ash and H. For PC2, the most influent parameter is humidity with whom is negatively correlated. From this grouping it is possible to appreciate how biomass vary depending on many factors. It is evident that woody biomass can vary their moisture content if they undergo a pelletizing process or not. Coffee is clearly an uncommon biomass with HHV and N higher than any other sample considered, as already seen in previous works (Colantoni et al., 2021). Furthermore, the coffee group shows an inner variability explained especially by humidity, this is probably due to the different kinds of blend produced with many sawdust percentages which bring to the moisture content decrease. Close to the woody pellets are placed the hemp samples that, despite the different nature respect arboreal biomass, have comparable composition and energetic yield. Hemp is therefore confirmed as feedstock of interest for many purposes such as textiles, pharmaceutic and energetic (Qamar et al., 2021; Rheay et al., 2021; Vandepitte et al., 2020). Like all herbaceous and straw species, hemp presents higher ash production in combustion, but if compared to the other straw samples, the amount is irrelevant.

Through the hierarchical cluster analysis (Fig. 3) using the Ward's minimum variance method are finally individuated four groups on which have been based the subsequent modeling evaluations. Principally, the arboreal biomass is divided in chipped and pelletized, while the SCG and straw biomass form other two distinct groups. Comparing such results with the trends shown through the ultimate analysis, three different linear models are proposed to better understand the link between composition and heating value in many kinds of biomass.

3.3. Correlations and modeling

From the compositional analysis it has been possible to fix a model for the HHV estimation for the biomass considered. Usually for statistical analysis, ordinary least squares (OLS) are mostly used and the fit quality evaluation is made by the coefficient of determination (COD) R^2. However the RQ models are more robust since they permit a more complete analysis of the conditional distribution of a variable depending on many predictors (Ranganai, 2016).

Despite the R^2 isn't properly used for quantile regression models, which are based on median or other quantiles, its calculation strengthens anyway the models built on the ultimate analysis and resumed in Table 2.When the complete dataset is considered, a strong correlation (R^2=0.85) is indicated for the Eq. (1). This model shows the smallest MBE, indicating a reduced systematic error to under and over forecast, but high MAE and hence higher forecast errors magnitude (Table 2).

Focusing deeply on the different groups identified through the PCA analysis, different models can be proposed for the estimation of HHV from the ultimate analysis. Since SCG has shown a relation between ultimate analysis and HHV closer to the herbaceous plant, the dataset has been divided into two groups: herbaceous and arboreal. Two different regression models are applied to these sub-datasets and the equations are resumed in Table 2.

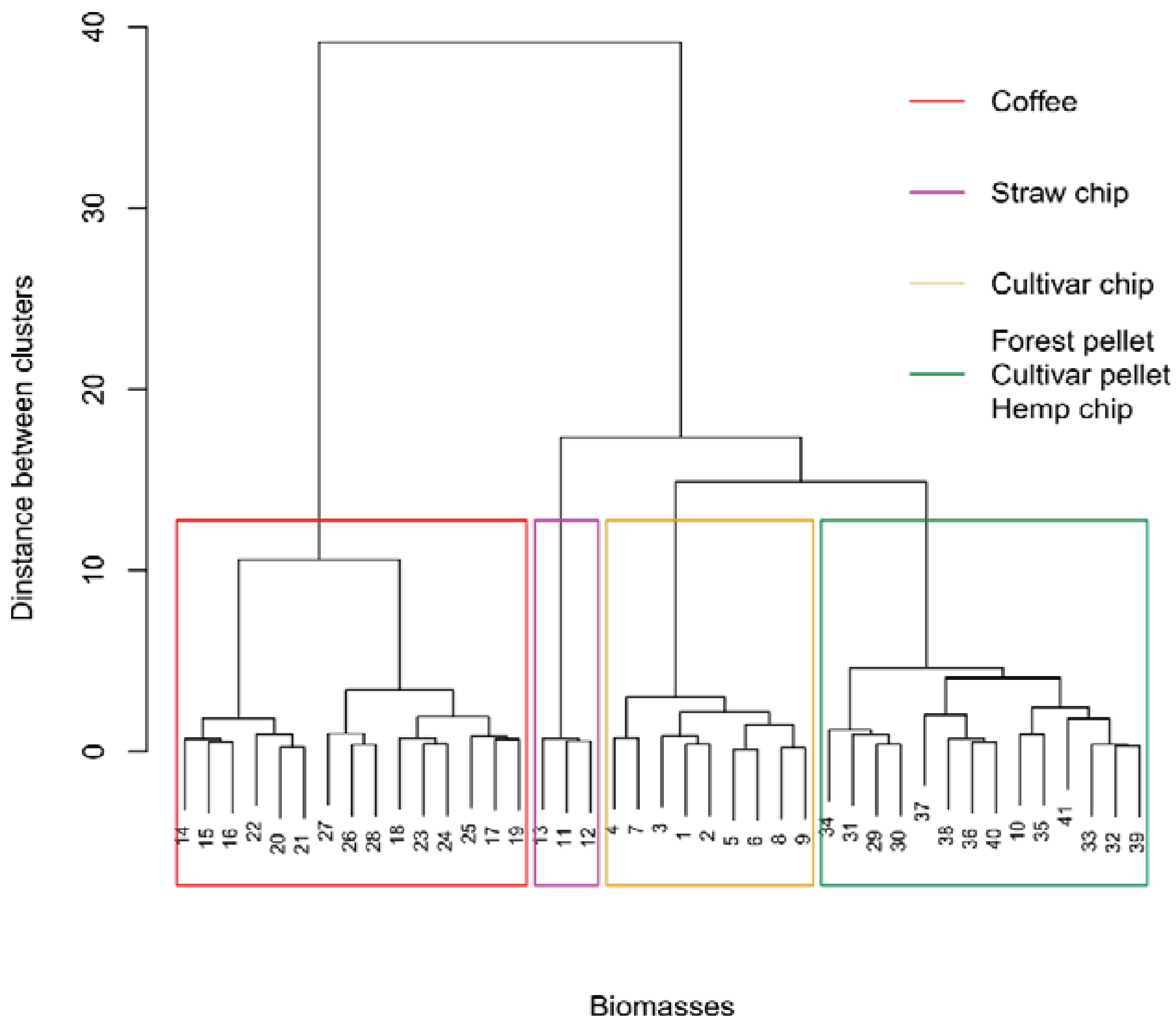

Fig. 3. Ward hierarchical cluster analysis of the biomass

Table 2. Models and relative accuracy parameters

Group	*Model*	*R^2*	*RMSE*	*MAE*	*MBE*	*Eq*
Complete	*HHV = 0.14C + 1.22N - 0.16H + 11.81*	0.85	0.1	0.58	0.01	*(1)*
Herbaceous	*HHV = 0.38C + 1.65N + 0.37H - 2.64*	0.96	0.06	0.38	0.02	*(2)*
Arboreal	*HHV = 0.08C - 0.49N - 0.03H + 14.93*	0.51	0.2	0.23	0.07	*(3)*

The higher variability in compositional analysis shown by arboreal species (Fig. 1) is reflected in the model quality too; for this group the smallest coefficient of regression R^2 has been calculated. Furthermore, such variability is detected by the RMSE too, which indicates the presence of large errors in the forecast (Table 2). The quantile regression fitted for herbaceous resulted the most accurate, with the smallest errors (RMSE = 0.06). When the calculated and predicted HHV values are compared, it can be seen that the plotted values are close to the curves of HHV estimated-HHV real, indicating good correlation accuracy (Fig. 4). In particular (Fig. 4), four quantile regression lines, in addition to the medians in bold, have been estimated for four values of τ (0.1, 0.25, 0.75, 0.9) for each model proposed. The same graph shows in blue the quantile regression lines for the herbaceous group, in black the arboreal ones, and in red the complete dataset regression lines. The lines estimated through quantile regression include almost all points on the graph.

Eq. (2) seems to be more accurate compared to Eq. (1) and (3) considering the presence of more outliers produced by the latter. In the upper-right corner of the graph are distinguishable coffee HHV values confirming the high energetic power of this matrix; in the middle part of the graph are present mostly arboreal species with some introgression of other herbaceous species, principally hemp; in the low-left corner the three straw biomasses bring out their lower predisposition to energy exploitation.

Many empirical correlations have been studied to predict the HHV from elemental composition, mostly for coals and other hydrocarbon fuels (e.g., biomass, char, oil) as well. Since it is well established that carbon and hydrogen contribute significantly to the biomass energy potential (Sheng and Azevedo, 2005), these two constituents are taken into account deeply. When hydrocarbons are evaluated it's known that a higher H content brings to higher HHV; saturated hydrocarbons are the simplest of the hydrocarbon species, they are composed entirely of single bonds, saturated with hydrogen and show higher HHV respect the unsaturated species with stronger bonds (Demirbas et al., 2018). For lignocellulosic biomass, the same reasoning can't be valid. In literature is confirmed that a positive correlation exists between C and HHV, while for hydrogen and HHV a clear trend isn't always observed (Jenkins M. et al., 1998).

In Sheng and Azevedo (2005), for example, the positive correlation observed between H and HHV is limited to a slight trend visible from data plotting without any statistical confirmation. In the present study, a positive correlation between C and HHV is observed (Fig. 5c) (Spearman: $\rho = 0.74$), but when H is considered (Figs. 5 d-f) , contrary to what is expressed in other works in literature (Mateus et al., 2021) a negative correlation (Spearman: $\rho = - 0.64$) can be observed (Fig. 5f). This behavior is strongly driven by SCG, which presents low H content and high HHV, differentiating itself from the other biomass considered in the models found in literature. Moreover, if we consider all biomass except SCG, the trend between H and HHV is negative tending to 0 (Spearman: $\rho = -0.07$), showing an absence of correlation between these two variables (p-value = 0.72). H content and HHV of arboreal species isn't correlated (Spearman: $\rho = 0.05$) (Fig. 5d), while only herbaceous species, including SCG, showed a negative correlation between the two parameters (Spearman: $\rho = -0.54$) (Fig. 5e).

When C-HHV correlation is examined, it can be noted that SCG better follows the trend shown by the herbaceous plants and the correlation between C and HHV for only SCG and herbaceous species increases till 0.92 (Fig. 5b). If only arboreal species are considered, the correlation decreases due to the higher variability of the compositional parameters. It is also noticeable that the quantile model fitted for only the arboreal species (Fig. 5a) underestimates the higher values of HHV and overestimates the lower ones.

This is probably due to the diversity of the biomass considered; for these biomass different storage methods have been used, furthermore the structural composition of tree biomass is usually considered more heterogenous with samples varying in bark and wood percentage and therefore in lignin and cellulose content (Barmina et al., 2013).

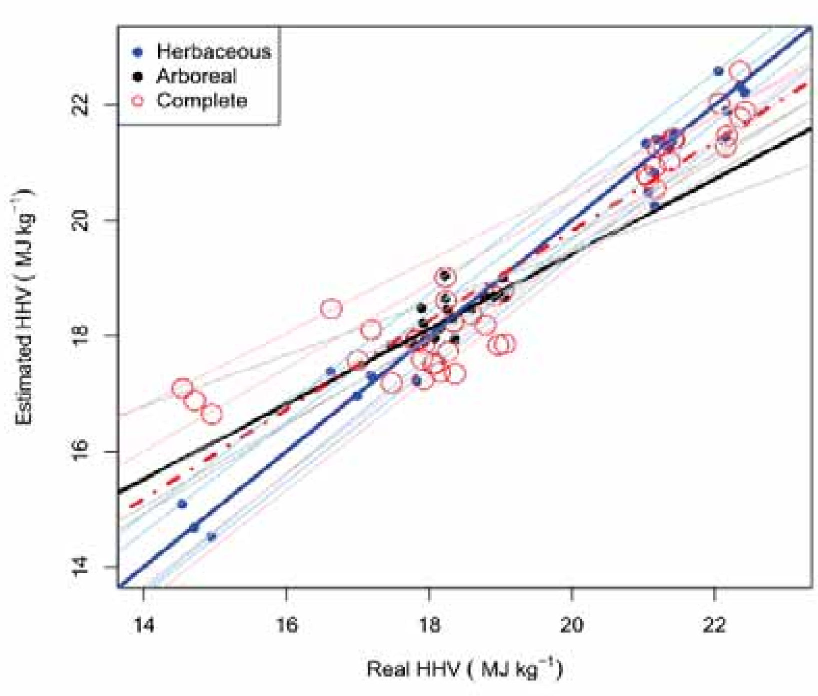

Fig. 4. Comparison between real and estimated HHV values for the three models

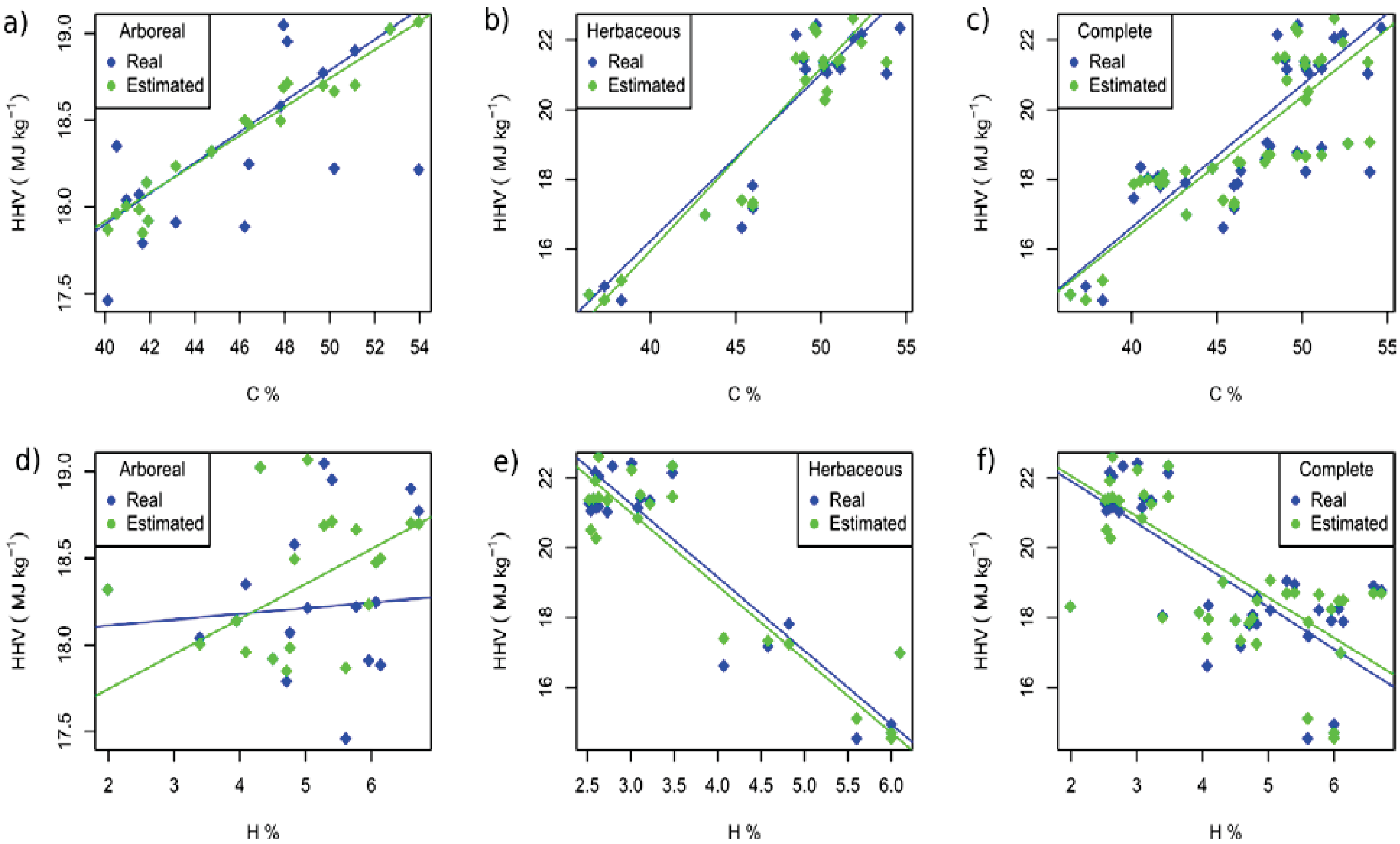

Fig. 5. Correlations between C and HHV for arboreal species (a), herbaceous (b), and for the whole dataset (c). Correlations between H and HHV for arboreal species (d), herbaceous (e), and for the whole dataset (f)

From the observations mentioned above, it follows that the relation between elemental composition and energetic yield isn't so homogeneous when the datasets comprehend many kinds of species with different physiology and physical structure. Studies that deepen and do not neglect such differences, are useful for a better comprehension of the processes involved in biomass energetic valorization, permitting better and wider modeling.

4. Conclusions

Through the PCA and cluster analysis, it has been possible to group the biomass and understand the energetic behavior depending on the ultimate and proximate analysis. In the two main groups highlighted (herbaceous and arboreal), linear quantile models have been applied for the prediction of HHV from compositional analysis (C, H, N). Such models show a good accuracy and confirm themself as a useful tool able to give information on biomass energy potential.

Arboreal species were marked by a higher variability in composition and the model fitted to them resulted less accurate, while Eq. (2) gave the best fit for herbaceous. Despite the typical differences between the studied biomass, Eq. (1) was able to give a good estimate of HHV.

In these models and calculations, SCG always shows the best energetic yield and the predicted values of each model concerning SCG are able to give extremely accurate values for this uncommon biomass. Straw biomass is the worst feedstock from the energetic point of view while arboreal and hemp place themselves between SCG and straw, but especially arboreal ones have already good and easy ongoing practices (harvesting, storage and drying) for their exploiting, thus resulting biomass easier to use in thermochemical processes.

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CONVERTING END-OF-LIFE PLASTIC WASTE INTO METHANOL: THE GASIFORMING™ PROCESS AS NEW, EFFICIENT AND CIRCULAR PATHWAY

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Abstract

The mixed plastic waste problem is becoming an important issue in scientific and technological communities in light of the environmental pollution caused by its poorly management. In this paper a new and efficient thermo-catalytic pathway to convert plastic waste into methanol is presented in its key features and global yields. The process has been mainly developed in silico using Aspen HYSYS V10 with support from experimental data where simulation could not provide reliable information such as the gasification step. Consolidated kinetic models are used both for the reforming and methanol synthesis steps, while the pre-reforming reactor is simulated at the thermodynamic equilibrium. The temperature, pressure, and mass flow balances of the system are reported alongside some of the most important key performance indicators for reforming (methane slip) and methanol synthesis (SN ratio).

Key words: circular economy, methanol, plasmix, plastic wastes, process simulation

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1. Introduction

Worldwide plastic production in 2017 was estimated at 348 million tonnes (PMERG, 2018) with a strong rising trend that has seen the rate of production rise from 202 million tonnes in 2002 up to 368 million tonnes in 2019 with no signs of slow down.

The total European demand in 2019 amounted to 50.7 million tonnes, with packaging applications consuming 39.6% of this figure, the construction (20.4%) and the automotive (9.6%) sectors following as the main plastic consumers in Europe. However, while the expected turnover of plastics in the construction and automotive sector could be qualitatively guessed to be in the order of years, the life spawn of a packaging application is typically very short and exhausts its purpose after a single use. These large volumes of waste generated within a short time have led to significant dispersion of plastic waste in the environment (Ilyas et al., 2018) leading to a new set of pollution issues concerning, in particular but not limited to, marine pollution (Jambeck et al., 2015). The packaging sector, being the most important one in terms of yearly plastic waste generation, is characterized by a specific subset of polymers.

These polymers are: Low Density PolyEthylene (LDPE), Linear Low-Density Polyethylene (LLDPE), Medium Density PolyEthylene (MDPE), High Density PolyEthylene (HDPE) which will be referred to simply as PE from now on, PolyPropylene (PP), PolyEthylene

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Terephthalate (PET), while combined PolyStyrene (PS) and its Expanded variant (EPS) make more than 85% w/w of the total packaging plastic demand.

The same distribution can be seen in post-consumer plastic waste in Table 1. The end of life of this waste mixture has drastically changed in recent years spurred both by European endeavours for a more sustainable economy, synthetized in the European Green Deal and in the EAP for 2030, and by China's 2017 National Sword policy which imposed stricter restrictions on recyclable plastics imports and drastically reduced the country's imports. This led to a reduction of recyclable plastic exports outside the EU by 39% from 2016 to 2018 making available for recycling further 29.1 million tonnes of collected plastic waste. Of this figure, only 32.5% was recycled and brought back to the market as a consumer product. Energy recovery is still the primary treatment method for plastic waste, being used on 42.6% of the waste.

The residual plastic, about 7.2 million tonnes, has no current application and is destined to landfill. This numbers vary greatly depending on the considered country, with landfill restrictions playing a major role in the split between landfill and energy recovery as shown in Fig. 1. The current primary recycling method used at industrial level is melt blending, popular due to its cheap, large-scale, solvent free nature and relatively extensive range of plastics to which it can be applied (Schyns and Shaver, 2021). This technique is applied through an extruder to induce thermal softening and plasticization of the polymeric waste and extrude the material into new pellets. The thermal treatment of the plastic over time will lead to degradation of the polymeric chains and loss of mechanical performance, which will be exacerbated by the presence of contaminants in the polymeric matrix.

Table 1. Mass composition of post-consumer plastic waste in Italy as reported by COREPLA in 2018 (COREPLA, 2019)

Polymer	*Weight fraction %*
PE	40
PP	25
PS	15
PET	7.5
PVC	2.5
Others	10

When different large enough polymers are mixed their Gibbs free energy will disfavour their blending, causing phase separation that will lead to very poor mechanical performance of the resulting mix (Flory, 1953). Due to inefficiencies in the sorting of the waste and accumulation of contaminants only a limited number of mechanical recycling cycles is possible (La Mantia et al., 2017).

The growing pressures towards the management of plastic waste have pushed towards new pathways that could make use of the portion of plastic waste currently destined to incineration and landfill to make new consumer products. The elemental composition of plastics, strongly resembling that of a crude oil vacuum distillation residue from the point of view of physical properties, while being relatively rich in hydrogen with a known aromatic content, makes the feedstock interesting as a crude oil alternative, also considering that the largest European plastic users (Germany, Italy) also lack this natural resource. For these reasons chemical recycling pathways have started to attract a lot of attention in recent years.

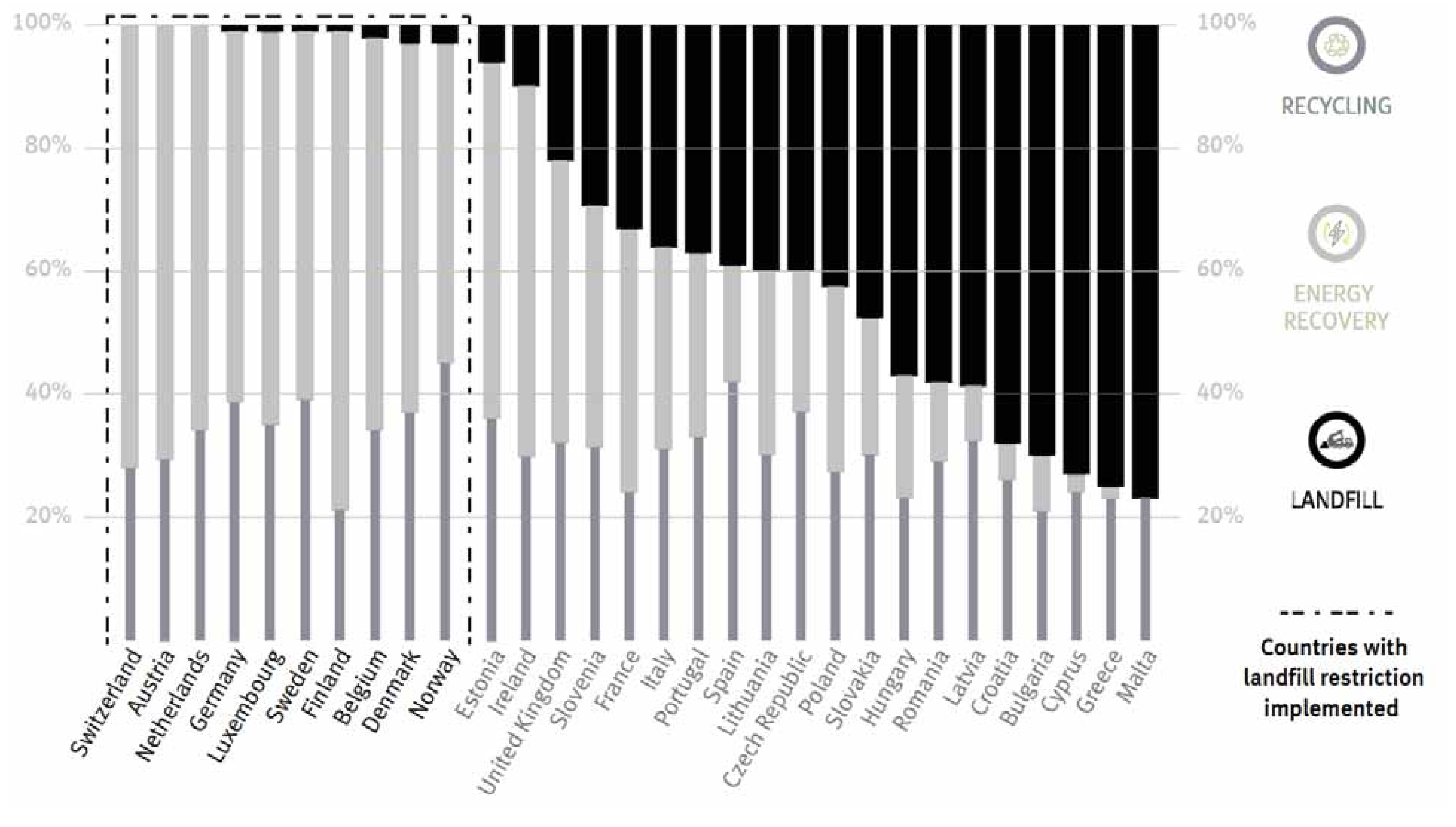

Fig. 1. End of life of plastic waste in EU countries (PMERG, 2018)

The current focus is on Pyrolysis to produce fuel gas and synthetic fuels (Encinar and González, 2008; Onwudili et al., 2009; Wu and Williams, 2010; Ranzi et al., 2016) with positive effects on global emissions with respect to incineration (Quantis, 2020). The process itself, being endothermic, necessitates for important energetic inputs which constitute an important part of the footprint of these plants. Another chemical thermal treatment is based on gasification techniques, typically implemented in fluidized bed reactors with similar designs to those currently used for biomass (Wu and Williams, 2010; Lopez et al., 2018).

Plastic gasification plants of industrial scale are not yet operative, however experimental campaigns have been carried out to evaluate feasibility and yields of the process. Arena et al. (2010) investigated yields at different temperatures and with various fluidizing supporting agent of different synthetic plastic feedstocks as well as sorted plastic refuse waste. An extended review on plastic waste pyrolysis, steam gasification and co-gasification of plastic waste with biomass and coal was carried out by Lopez et al. (Lopez et al., 2018) showing that plastic waste gasification plants at the moment are still not diffused, and how they differ from biomass and coal mature technologies. The most important difference shown by Ahmed and Gupta (2011) and Lopez et al. (2016) concerns the fact that char gasification is not the limiting kinetic step in plastic gasification as it is the case with biomass and coal and consequently limited solid residue is present.

Moreover, as seen in Pinto et al. (2003) by combining gasification with a fixed bed of Dolomite and Ni-Alumina it is possible to reduce residual tar to negligible contents. Similar results are obtained using commercial reforming Ni catalyst operating at a temperature up to 600°C downstream of a spouted bed by Lopez et al. (2015), which also showed improved hydrogen yield. A similar approach was used in this simulated work to deal with possible residue tar. The patented design is applied to achieve gasification of the plastic waste with low CO_2 yield in mild conditions approaching optimal conditions for Methanol production.

2. Material and methods

Inspired by the design of the Texaco process for asphalts gasification the Gas-forming process applies a similar concept to plastic waste. The layout shown in Fig. 2 involves the pre-treatment stages of the plastic waste up to their gasification and preliminary reforming. The waste is first milled in mechanical unit (Unit 1) operating in ambient conditions, reducing the characteristic dimensions of the plastic waste to a diameter of a couple centimetres. These pellets are then immersed in two successive tanks with a different solvent in each. The first solvent is water in which PP, PE and most of the PS will float, while PET and PVC will sink. In a second tank brine with a density of 1350 kg/m^3 is used, PET and rigid PVC will still sink while flexible PVC will float, this fraction of PVC, being the majority of polymer in the mix, is removed while the PET PVC mixture is sent is collected at the bottom (Unit 2). The collected PET and PVC are washed to remove deposited salts (Unit 3) and then sent, alongside the other polymers collected as floating material in the first sedimentation tank, to the pre-melter (Unit 4). In Unit 4 the plastic mix is heated at a temperature of 300°C. At this temperature, the mixture will behave as a liquid and partially react decomposing in light components. The residual PVC in particular will release chlorine as HCl (Ranzi et al., 2016) which can be removed from the system alongside a minor quantity of light components which will be sent to gas treatment. The liquid plastic mix is sent to a second melting tank (Unit 5) where the temperature is further raised to 350°C to improve viscosity. Light hydrocarbons released in this tank are collected and sent to the gasification chamber while the liquid is sent to a pump (Unit 6) to be pressurized at 15bar for atomization. Finally, the plastic melt is mixed in a twin fluid atomizer with mid pressure steam and pure oxygen and ejected through a nozzle in Unit 7 losing up to 5 bars in the atomization step.

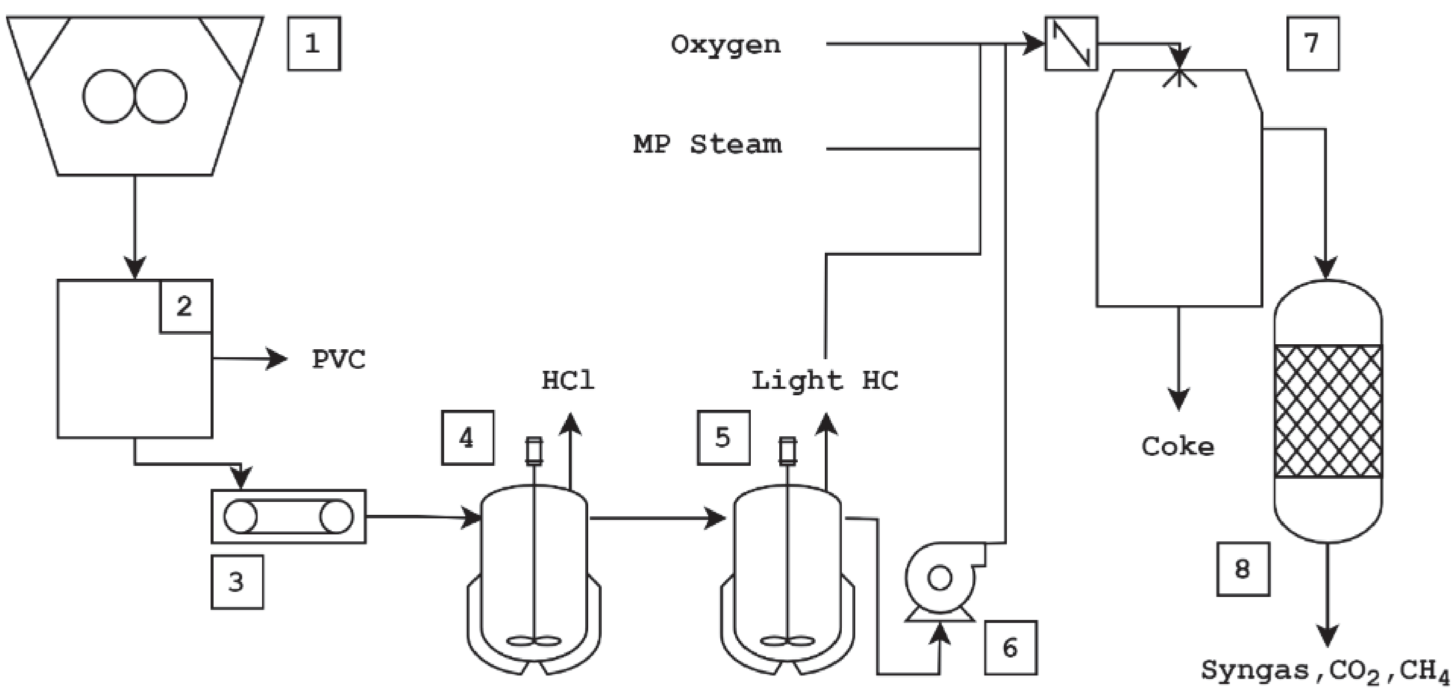

Fig. 2. Gasiforming process layout

In the gasification chamber a series of reactions degrade the polymer mix to hydrogen, carbon monoxide, carbon dioxide, methane, ethane, propane, ethylene, toluene, benzene, and carbon coke. Carbon coke is collected at the bottom of Unit 7 while the gaseous stream, still rich in heavy and aromatic hydrocarbons is sent to a pre-reforming unit (Unit 8) where ethane, propane, benzene, and toluene are degraded to methane and syngas. The richness of the syngas in CO_2 coming from the gasification makes the feedstock suitable for methanol synthesis.

The syngas is first mixed with more medium pressure steam and fed to a steam reforming unit (Unit 9) where methane is converted to syngas. Steam is added with a H_2O/CH_4 ratio higher than 3 due to the difficult conversion and high methane slip in the reformer caused by the presence of CO and H_2 in the feed that further complicate the thermodynamically limited reactor (Farshchi Tabrizi et al., 2015); the same reason stands for the unconventionally low operating pressure of the unit. The residual heat in the output is captured by a series of exchangers and then fed to a flash (Unit 10) where the condensed water is removed before compression to 80bar (Unit 11). Typical pressures for methanol synthesis go from minimum values of 60bar up to 120 bar (Mäyrä and Leiviskä, 2018), the value of 80 bar was considered a reasonable middle operating point for adiabatic bed reactors operated with commercial CZA (Cu-Zn-Al) catalyst. A crucial optimization parameter for methanol synthesis is the Stoichiometric Number defined as Eq. (1):

$$SN = (H_2 - CO_2)/(CO + CO_2) \quad (1)$$

In the analysed system there was an excess of CO_2 which had to be removed. A patented system using physical adsorption with water (Unit 12) was applied to remove food grade quality CO_2 from the syngas, which was then sent to a two stage, intercooled, adiabatic methanol reactor (Unit 13) and finally to a distillation column as shown in Fig. 3.

In the current work a simplified simulation of the plant starting from Unit 8 is presented. The exclusion of the mechanical pre-treatment and melting phases is due to their relatively low complexity (Units 1, 3 and 6) and the lack of appropriate kinetics (Units 4 and 5) to make the simulation of that section possible in Aspen HYSYS V10. Unit 7 yields were found with two experimental campaigns in a fluidized bed reactor described in detail in Parrillo et al. (Parrillo et al., 2021). Moreover, PET and PS were not available for the validating experimental campaign in the desired quantities, so a synthetic mix of polymers was used to simulate the waste: 49% w/w HDPE, 49% w/w PP, and 2% EPS.

Finally, the steam generating capacity of the experimental plant was not able to provide more steam that the input used in this work, which represented an operating limitation of the experimental campaigns. During the experimental campaign, the gasification unit was operated at atmospheric pressure at a steady state average bed temperature of 785°C with air (instead of pure oxygen, which was not available). The feed consisted in 35 kg/h of plastic mix, 23 kg/h of oxygen, and 12 kg/h of steam. Several simplifying assumptions were made at this stage:

- Negligible effect of pressure on the system yield and product distribution, which is not correct (Li *et al.*, 2010), but was considered negligible for a 8bar difference and a preliminary feasibility stage.
- The yield of a fluidized bed reactor is not significantly different from the yield of the atomized reactor as both systems will reasonably reach thermodynamic equilibrium at the outlet (Silva *et al.*, 2019)
- Nitrogen is inert in the system and does not significantly influence the chemistry of the reaction. The presence of nitrogen will lower the partial pressure of the system and, for what said before, influence in a small extent the yields, this effect is considered negligible also in this case due to the low pressures of the system.

While these approximations introduce significant errors in the system due to unreliable predictions on the performance of the atomization chamber, they still represent a relatively accurate prediction of what can be obtained from a plastic waste mixture through gasification and are in line with other previous literature (Brems et al., 2013; Lopez et al., 2018; Ragaert et al., 2017).

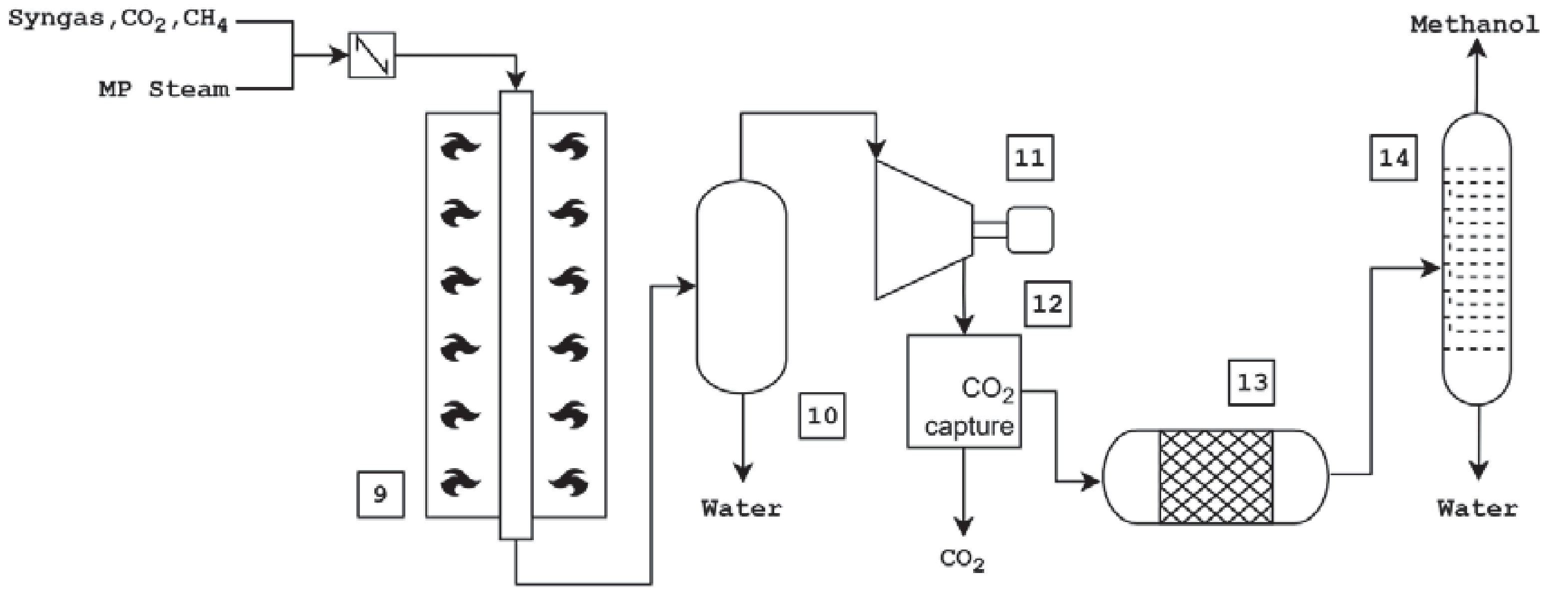

Fig. 3. Methanol synthesis from Gasiforming process

Moreover, this source of error is further dampened in its effects by the presence of a Gibbs reactor operating at 500°C after the gasification chamber. The purpose of this reactor is to degrade residual tar and favour the water gas shift reaction. Since the outlet of the Gibbs reactor will be at thermodynamic equilibrium the effect of pressure variation in the gasification chamber will be compensated for in this step.

The feedstock to the plant was normalized after removing nitrogen which cannot be tolerated in the system since it would require complex separation techniques. This stream was set at 10 bar and introduced in Aspen HYSYS V10 at 785°C. Flowrate was scaled to treat 1000 kg/h of plastic mix since this value is the target dimension for the experimental plant to be build and every flowrate was scaled proportionally leading to 1000 kg/h of plastic waste, 658 kg/h of pure oxygen, 344 kg/h of steam. From the experimental campaign negligible formation of solid was observed, while tars, represented in the simulation by naphthalene (Lopez et al., 2018), were present in significant amounts. Aromatics, especially benzene were also measured in significant quantities. The detailed composition of the gasification output is reported in Table 2.

Table 2. Normalized composition obtained from experimental campaign at 1 bar, 785°C

Component	***mol/mol***
Hydrogen	11.7
H_2O	24.4
Naphthalene	0.3
CO	8.0
CO_2	19.7
Methane	17.5
Ethane	12.5
Propane	0.4
Acetylene	0.5
Ethylene	2.0
Toluene	0.2
Benzene	2.8

This stream was used as an input in Aspen HYSYS V10 simulation. After being cooled at optimal temperature of 500°C in a process-process exchanger to generate steam, the hydrocarbon mixture is fed to a pre-reforming unit operated adiabatically (Christensen, 1996). The unit in HYSYS is simulated as a Gibbs reactor accounting only for thermodynamics, but this situation is considered in line with conventional pre-reforming operation (Christensen, 1996). The reactor results in an exothermic behaviour rising the temperature of the syngas at 597.5°C. While several endothermic reactions take place in pre-reforming units, the exothermic water gas shift reaction is also significant, and due to the higher concentration of water and carbon monoxide with respect to higher hydrocarbons an overall exothermic reaction is observed. Steam is added to the stream until the H_2O/CH_4 ratio is 4 and fed into a reforming unit at a inlet temperature of 422.5°C. The lower inlet temperature (typical value is 500°C) is tolerated here because of the low concentration of methane that gives the system more thermal inertia and makes it less endothermic. The steam reforming reactor is modelled as a PFR with Xu-Froment reaction kinetics with commercial Ni based catalyst (Xu and Froment, 1989) operated at a pressure of 899 kPa and at an outlet temperature of 900°C, achieving methane conversion of 92.2%, with an outlet H_2/CO ratio of 2.977. The high H_2/CO ratio is determined by the pre-reformer which consumes water to break down the heavy hydrocarbons while introducing further hydrogen in the stream components. The stoichiometric number is low (1.47) due to excess presence of CO_2. Before compression water removal is necessary. The stream is cooled down to 50°C while generating the medium pressure steam necessary for the reformer. Condense water is removed and the syngas is sent to a two-stage intercooled compression system to be pressurized at 80bar. After compression, the SN ratio is regulated using a patented CO_2 removal technique capable of removing 568.3 kg/h of CO_2 with a minimal loss of 0.71 kg/h of H_2 and 4.37 kg/h of CO and requiring 190.7 electrical kWh. The sweetened syngas, now having a *SN* of 2 is then fed to the methanol synthesis loop. Two PFR adiabatic reactors are used in series with an intermediate cooler. The first reactor is fed with syngas at 220°C (temperature at which the copper-based methanol catalyst is active) and the stream exits at 328.4°C in thermodynamic equilibrium. The second stage is still fed at 220°C but the output is at 301.9°C degrees due to lower conversion in the second stage. In both reactors Graaf kinetics for CZA catalysts are used (Graaf et al., 1988). The crude methanol mixture is cooled to 65°C by pre-heating the syngas feed to the first reactor and in an exchanger later. A flash at 77.4bar is used to separate the unconverted syngas, which compressed back at 80bar to recover the pressure drops, from the crude methanol that is collected and sent to a methanol distillation system.

The separation section is subject to another issue. Due to the kinetic scheme used crude methanol contains only methanol and water, which is not the case in actual methanol plants (Ross, 1986), where also higher alcohols and ethers are formed during synthesis. The yields of each depend on the specific catalyst and operating conditions of system. Assuming the simple case simulated is true, it makes the downstream trivial and 99.5% mol/mol Methanol can be distilled with a single 12 stage column with 99% component recovery. In a more complex case (Zhang et al., 2010) multiple columns are necessary to achieve high purity of methanol. The detailed Aspen HYSYS V10 flowsheet is reported in Fig**.** 4. The reported plasmix se feed consists in n-C30, which acts as a stand in for the polymer plastic mix to allow a gross estimate of the necessary duties for heating and pumping the material. In the Gasification Chamber sub-flowsheet, the experimental data is used to reconstruct the output of gasification.

3. Results and discussion

The simulation carried out for a preliminary investigation of the feasibility of methanol production from plastic waste showed interesting potentiality in its ability to generate 1.35 ton/h of 99.5% pure methanol starting from 1 ton/h of generic plastic waste. In Table 3 the material streams as simulated are reported in key positions in the plant. Several optimizations are being considered at this stage of development but were not implemented as new experimental campaigns are necessary to validate the behaviour of the pre-reformer and its ability to tackle the degradation of tars, which are thermodynamically unfavoured as the simulation shows, but the kinetics and the limits of HYSYS in predicting actual coke formation could lead to significant issues during plant operations and thus lower overall methanol yields.

The formation of solid residues in the gasification chamber is a significant concern despite not being observed in the two experimental campaigns currently performed in fluidized beds. This could lead to the formation of coke, in a best-case scenario, or an undefined ash with high carbon content. Both scenarios are not necessarily bad, since the design of the chamber can easily cope with solid particles and the formation of coke would lead to higher hydrogen content in the formed syngas, but they require changes in the plant design to account for possible solid entrainment. Moreover, the presence of unknown compounds and the naturally evolving nature of waste could involve the presence of unforeseen compounds in the stream. This issue is considered unlikely to be problematic in actual operations since waste collected over a large basin exhibits only marginal seasonal changes and is overall stable in composition. Vulcanized rubbers might introduce sulphur-based compounds in the system which are harmful to the catalyst of the reformer and pre-reformer, but rubbers are typically removed and collected in previous treatment stages of the waste since the presence of sulfurated compounds is harmful even in case of incineration.

A similar role might be taken by additives used in plastic manufacturing and contaminants of metallic nature which must be removed either prior to reaching the plant or in the in the melting units. The case of metallic residues being particularly easy as they can be separated by simple decantation once the plastic is liquefied. Finally, the melting phase effects on the properties of the plastic mix is subject to significant predictive errors due to the fact that the correlations used for the computation of viscosities and properties of the polymers in the mix (Cornish, 2012) are regressed on data that seldom comes near to the pyrolysis temperatures (T>250°C).

While there is significant margin for error there is also a really appealing yield of the plant made even more interesting by the role methanol can have in a hydrogen-based economy as a transition element.

4. Conclusions

The design of a plastic wastes to methanol process was shown and described in its most important features. While several issues require to be addressed in a manner not suitable for simulation and significant room for optimization and improvement is still present the yield showcased yield already makes a case for an interesting alternative to direct incineration of the plastic waste and pyrolysis.

Table 3. Temperatures, Pressures, and Flowrates measured in kg/h of each component in specific points in the plant reported in Fig. 4

	1	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*
T [°C]	350	500.0	597.5	422.5	50.0	21.4	301.9	34.0	65.0	52.6
P [kPA]	1500	999.0	999.0	899.0	899.0	8000.0	7740.0	200.0	200.0	150.0
H_2	0.0	18.4	15.5	15.5	271.5	270.7	778.8	0.5	0.0	0.0
H_2O	344.1	343.0	69.8	3096.5	55.6	2.0	138.3	137.2	136.3	0.4
naphthalene	0.0	29.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO	0.0	174.3	383.1	383.1	1266.9	1262.6	2356.7	2.3	0.0	0.0
CO_2	0.0	674.9	844.6	844.6	1198.4	641.9	2397.2	79.1	8.3	8.3
CH_4	0.0	219.2	689.4	689.4	53.5	53.5	530.8	1.9	0.0	0.0
C_2H_6	0.0	292.7	0.5	0.5	0.5	0.5	4.4	0.0	0.0	0.0
C_3H_8	0.0	15.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C_2H_2	0.0	10.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
C_2H_4	0.0	43.9	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0
Toluene	0.0	13.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Benzene	0.0	167.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
O_2	658.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CH_3OH	0.0	0.0	0.0	0.0	0.0	0.0	1485.1	1402.9	1357.6	1344.0
PE	490.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PP	490.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
PS	20.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TOT	2002.7	2002.8	2002.8	5029.4	2846.3	2231.2	7691.4	1623.9	1502.2	1352.6

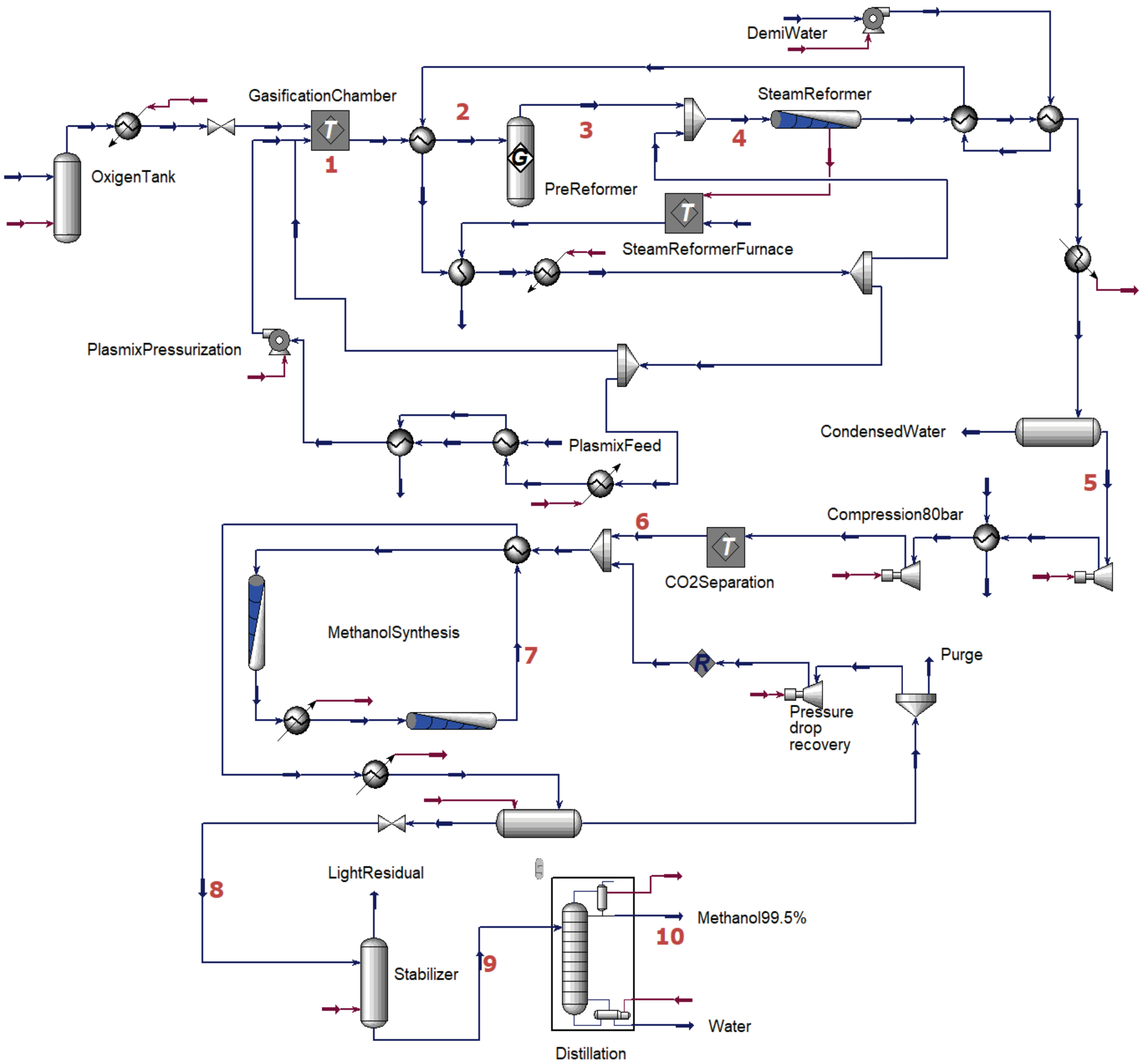

Fig. 4. Plant layout in Aspen HYSYS V10

The choice of methanol as a product is related to the significant presence of CO_2 in the system, but the availability of low-cost syngas from plastic waste could lead to several new pathways to commodity chemicals such as ammonia (enriched air gasification would be feasible in this case), dimethyl ether (further CO_2 utilization) and direct hydrogen production (simplest plant design with WGS reactor after the reformer).

This solution is even more interesting in realities like those typical of Europe where plastic collection is well developed, the densely populated urban areas produce a reliable and continuous amount of waste, hydrocarbon natural sources are not present, but methanol is in high demand for its role as gasoline additive.

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ANALYSIS OF WIND TURBINE PERFORMANCE, OPTIMIZATION, TECHNICAL-ECONOMIC AND ENVIRONMENTAL FEASIBILITY

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Abstract

To make wind energy more usable, a new prototype of high efficiency wind turbine will be developed in this work. For this purpose, a new proprietary mathematical model will be implemented, for the design of wind turbines and new design concepts, in order to maximize the energy capturing capacity of the wind turbine. Currently the numerical simulations for predicting the performance of a wind turbine are carried out with 3D CFD programs (Computational Fluid Dynamic) characterized by high reliability, but which at the same time require significant resources and high calculation times. As an alternative to CFD codes, both the scientific and industrial communities use one-dimensional calculation models. These codes, if properly implemented, can provide sufficiently correct results, but characterized by modest resources and very short calculation times. All this allows to carry out numerous simulations runs in reduced times, reaching the optimal configuration of the turbine in a few minutes. An environmental analysis of the proposed technological innovation, measured making use of the most suitable widespread environmental reporting tools, is then proposed and recommended, through an inventory of the emissions of environmental impacts, according to a Life Cycle Assessment perspective. An evaluation of the competitiveness of the new technology has to be implemented, in comparable contexts, to verify its performance in terms of economic and environmental sustainability. Finally, a cost-benefit verification of the investment and its socio-cultural impact is also necessary, considering the production process of the turbine and its implementation, in view of the decarbonization of the economy too.

Key words: CFD, economic analysis, energy, environmental impacts, wind turbine

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1. Introduction

Nowadays, at both academic and industry level, the most used mathematical model in order to fulfill the fluid dynamic design of wind turbines is the one based on BEM (Blade Element Momentum) Theory (Buhl, 2005; Corten, 2001; Lanzafame and Messina, 2007; Meyer and Kroger, 2001; Moriarty and Hansen, 2005), founded on Glauert theory (Glauert, 1926). Although not offering the accuracy of CFD (Computational Fluid Dynamic) codes, the mathematical model offers several benefits, among which the calculation speed (each numerical simulation is carried out in a few seconds) (Lanzafame and Messina, 2007; Lanzafame and Messina, 2010).

Without going into the details of the mathematical calculation, once the aerodynamic profile to be used in the wind turbines' production has been selected in view of the experimental data regarding lift and drag, the traditional mathematical model determines the wind turbine's twist by imposing an angle of attack along the entire turbine which is equal to the one maximizing the lift and drag ratio. Additionally, during the design phase, a certain

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wind speed is selected, in order to create operating conditions toward power and torque maximization.

The aforesaid process might be implemented when planning a wind turbine able to be employed in several types of installation sites, characterized by different wind speed distributions. Instead, when the goal is the designing of a wind turbine for a specific site, the aforementioned process can not represent the optimal combination of decisions to achieve the maximum level of energy produced in a single year (AEP – Annual Energy Production). Thus, the yet described new designing method becomes essential when a wind turbine must be used with low wind velocity.

In this paper, we will present the methodology that should be adopted in the perspective of AEP maximization in the context of an installation site characterized by limited wind. Moreover, several designing strategies will be employed emphasizing how each one of them increases the AEP in comparison to the energy produced when following the traditional method. We will also introduce the main methodological guidelines concerning the way for taking into consideration the economic and environmental aspects, their impacts and their measurement in the framework of green energy production.

2. Material and methods

The procedure followed for the design of the wind turbine blades object of this work is to:

- establish a design wind speed (called v_0);
- maximize the efficiency for the speed v_0;
- evaluate its performance with variable wind speeds.

As already mentioned, in the literature Gash and Tewele, 2002; Sphera, 2009), there are indicators according to which the design of wind turbine blades must be performed for values of the angle of attack $\alpha=\alpha_{max}$, an angle that maximizes the lift/drag ratio. Following these indicators, the first value of α that was entered as input to the code for the design was precisely α_{max}. In order to find the optimal operating conditions (maximum AEP) a turbine with three blades (N_b), with a tip radius (R_1) equal to 2 m and a hub radius (R_b) of 0.4 m of has been studied. The radial sectors (s) have been set equal to 20 and the wind speed (v_0) equal to 4 m/s, equal to the average speed of the histogram characterizing the installation site shown in Fig. 1. For the wind turbine study, two numerical codes were used (Lanzafame and Messina, 2007), and a value of $\alpha = \alpha_{max}$ (α is the angle of attack, and α_{max} il the angle of attack which maximizes the lift to drag ratio) which for the chosen profile (S809) is equal to 6.16°, has been set. For the determination of the chord, reference was made to the following equation (Eq. 1) based on the still valid theory proposed by Schmitz (1955).

$$c = \frac{1}{N_b} * \frac{16 * \pi * r}{c_L} * \left[sin\left(\frac{\phi}{3}\right)^3 \right] \quad (1)$$

where: Φ is the angle between the air foil chord and the plane of rotation and c_L is the air foil lift coefficient.

Lift and drag experimental coefficient have been taken from scientific literature (Jonkman, 2003) and (Lindeburg, 2003), and have been interpolated as report in Lanzafame and Messina (2007). While the twist value (Θ) was calculated using the following formula (Eq. 2):

$$\vartheta = \phi - \alpha \quad (2)$$

where: α is the angle of attack.

This code outputs the twist values at certain radial position. In order to derive a mathematical function for the twist, a logarithmic polynomial of the fifth order (solid line of Fig. 2) was used to interpolate all the punctual data output from the design code. The logarithmic polynomial has the functional form of:

$$\Theta(r) = a_0 + a_1 lnr + \ldots + a_5[ln(r)]^5,$$

where a_i are constants.

Subsequently, this function was included in the code for the evaluation of performance in off-design conditions. Starting the simulation, the power curve and the power coefficient shown in the graph of Fig. 3 were determined, the graph shows that the c_p is high for values close to the design speed, but decreases rapidly for different values.

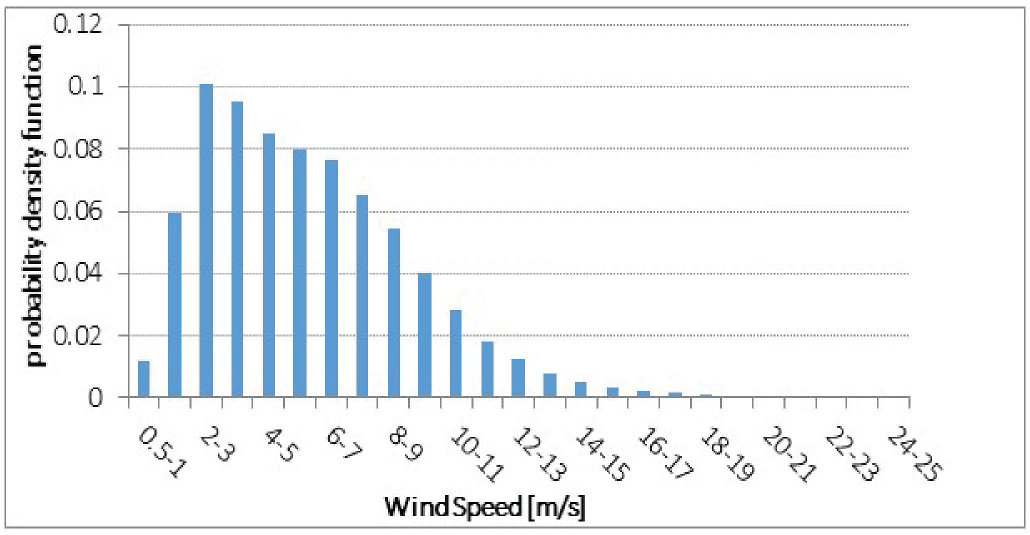

Fig. 1. Wind frequency distribution histogram (Location "Piana di Catania")

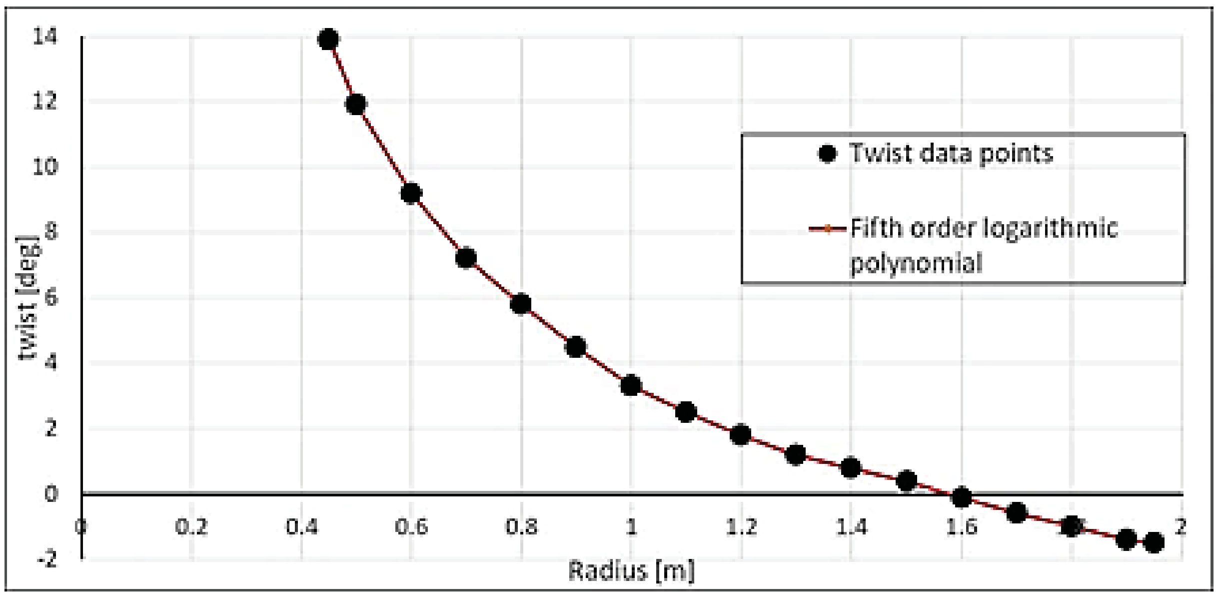

Fig. 2. Blade Twist

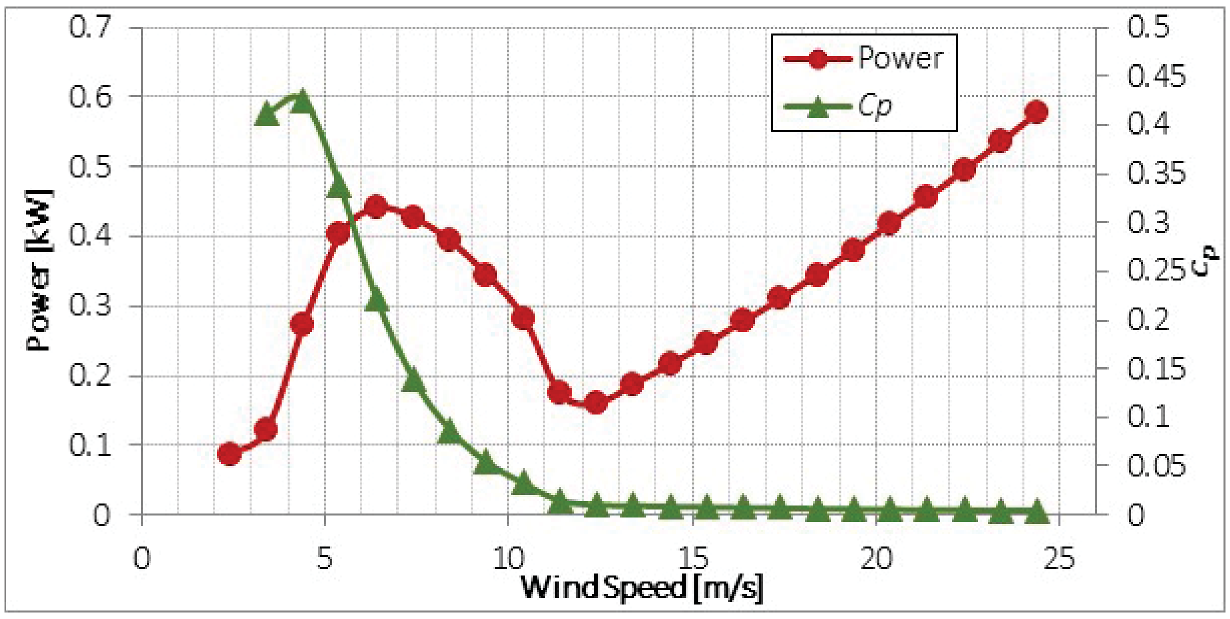

Fig. 3. Wind turbine Performance (P e c_p) designed with $\alpha = \alpha_{max}$ and $v_0 = v_{med}$

Knowing the power curve and comparing it with the wind histogram of the installation site, the AEP was calculated with the following equation (Eq. 3):

$$E_w = \sum_{j=1}^{N'_B} P_w(m_j) f_j \Delta t \quad (3)$$

where: N'_B are the sectors of width w with midpoints m_j, and with frequency f_j.

The graph in Fig. 4 shows the power curve superimposed on the frequency histogram created by collecting wind measurements at the installation site for a year (Δt = 8760 h), with N'_B = 26, w = 1 and m_j = (j-0.5). With these parameters, the estimated AEP was equal to 1674 kWh/y.

Twist correction

From Fig. 2, near the tip, the designed twist has negative value. The torque of the wind turbine depends from a tangential force directed as the rotational velocity. At the radius where the blade twist has negative value, the tangential force can change direction and generate negative torque (only for some sector of the blade). This phenomenon leads to very low c_p values and a decrease in power. Observing Fig. 3, it is possible to notice a strong decrease in power for values between 10 m/s and 15 m/s. To overcome this drawback, the twist of the blade has been modified, and near the tip the twist value has been increased. To obtain a new improved twist, the following correction (Eq. 4) was applied (Lanzafame and Messina, 2010):

$$\vartheta(r) = \sum_{i=0}^{5} a_i \cdot [\ln r]^i + x \cdot r^2 \quad (4)$$

3. Results and discussion

Following the modification reported in Eq. 4, a power curve and a new power coefficient were obtained. Fig. 5 shows that the curves for v <7 m / s remain substantially unchanged with respect to the previous ones, while for v> 7 m / s, a considerable gain is obtained both in terms of power coefficient (c_p) and Power (P).

This is visible in Fig. 5 where the new power and power coefficient curves were compared with the previous ones. Applying Eq. (3), the evaluation of the energy produced annually by the turbine, designed for α=6.16, v_0=4 m/s and with the geometry of the blades characterized by the new twist (x=1.4), an AEP = 2166 kWh/y was obtained.

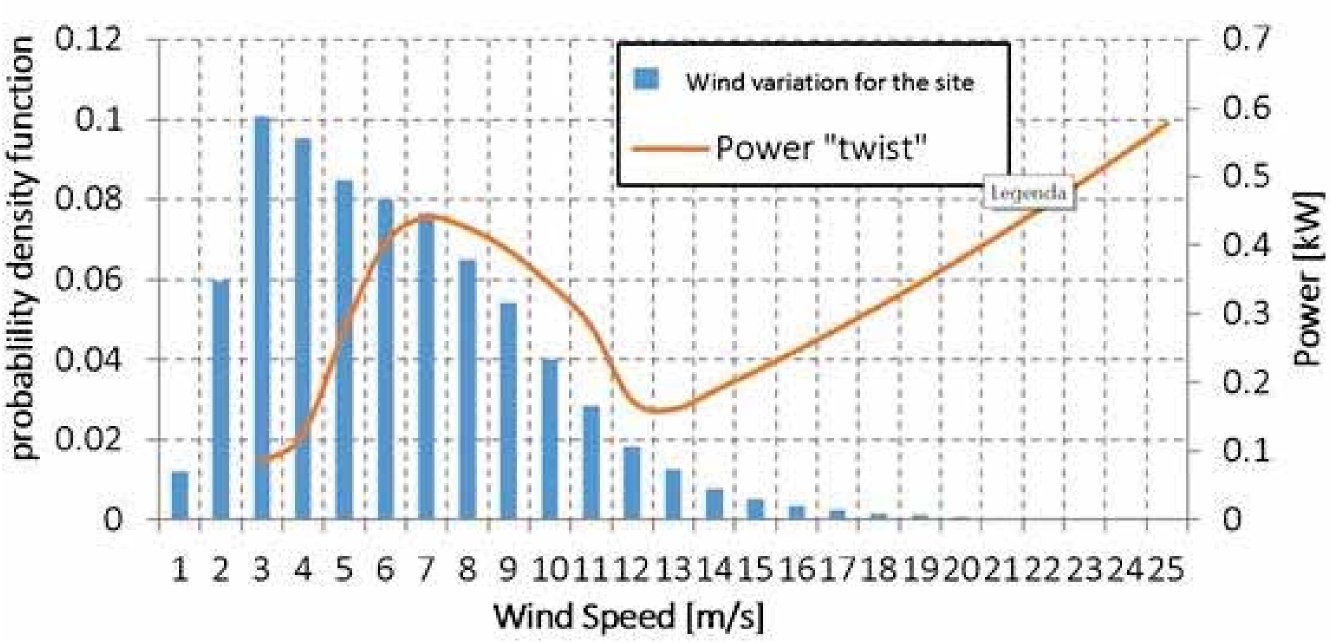

Fig. 2. Wind histogram for site and power curve for WT with $\alpha = \alpha_{max}$ and $v_0 = v_{med}$

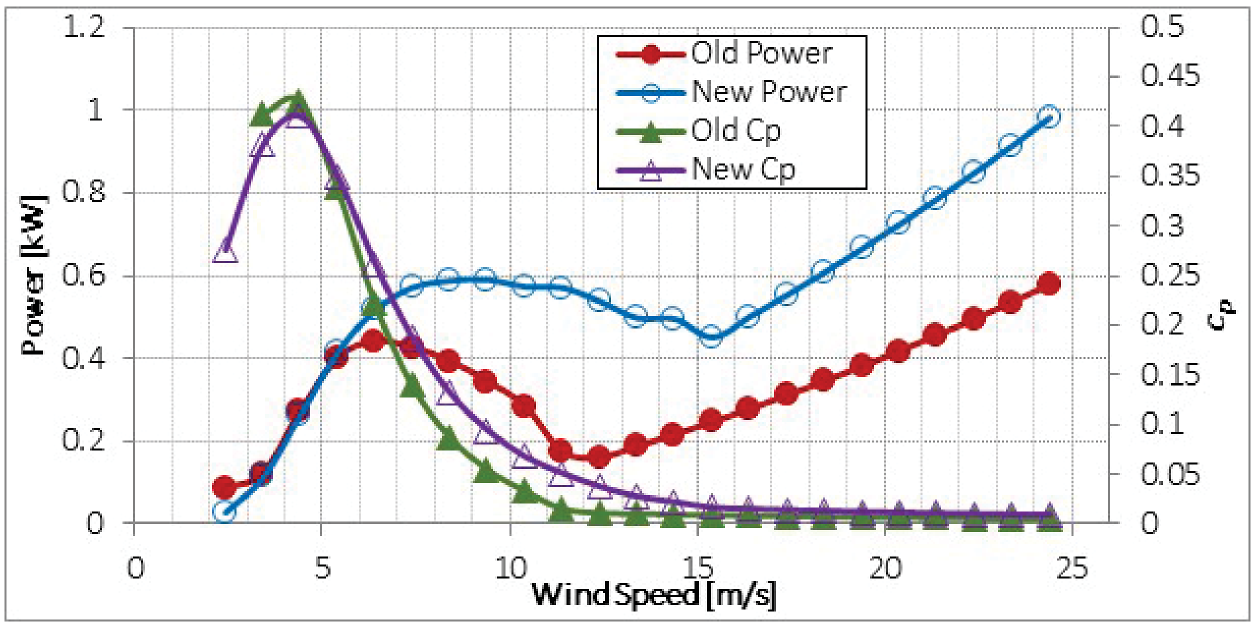

Fig. 5. Comparison between old and new power curves and power coefficient

This means that the twist correction would lead to a higher production of about 492 kWh/y thus obtaining an increase in annual production of just over 30%. To maximize the annual energy production, it is necessary to individuate the optimal values of α, v_0. This may be achieved by employing the calculation procedure previously described to calculate AEP. In a first phase, with the value of $\alpha = \alpha_{max}$ constant, varying the value of v_0 within the interval between 4 and 13 m/s with steps of 1 m/s. After the optimal value for v_0 [$v_{0\ opt(1)}$] was identified – which in this specific case is equal to 10 m/s and for which the AEP has its maximum value – the value of $v_0 = v_{0\ opt(1)}$ has been taken constant and re-runned the simulations allowing the variations of α in the range between 4° and 8°. Also, in such cases the AEP values have been calculated for each value of the angle of attack and without making corrections to the twist.

In conclusion, the point characterized by values of $\alpha = 4°$ and $v_0 = 10$ m/s (twist correction $x = 0.2$) is the optimal point for the planning of a wind turbine that would have an estimated yearly production of 8526 kWh/y. Fig. 6 represents the rotor optimized for the AEP maximization in sites characterized by limited wind. Fig. 7 displays the aerodynamic profile S809 and the twist of the wind turbine rotor. Figs. 8 and 9 display the optimize wind turbine power curve and the optimized wind turbine power coefficient.

Fig. 6. 3D representation of the designed wind turbine rotor

3.1. Economic and environmental aspects

After the assessment of the technical aspect's optimization, it is crucial to examine the economic worth and the environmental impact of the project. At this end, first of all it is necessary to compute the present value of the project cash flows, namely the temporal distribution of its monetary outflows and inflows, and the time horizon of the analysis, that is the economic life of the plant. Actually, we need also to consider several scenarios, by hypothesizing a total private or a partial public funding, through financial subsidies.

The assessment of the outflows seems pretty easy, as we know the costs of all the components of the plant, and the periodical maintenances required. Conversely, more complex is the inflows appraisal, due to the energy price dynamics, the plant obsolescence, the long-lasting economic life of the plant, and so on. In any case, we need to calculate the most important economic and financial indexes (Net Present Value, Internal Rate of Return, Payback Period), suitable to analyse the profitability of the project (Munda and Matarazzo, 2020). This kind of additional analysis is actually very important for the real fulfilment of the plant

Our study becomes even more complex if we aim to analyse the project also from the public decision maker's perspective. Indeed, in such a case, we need to explicitly consider also the economic, social, and environmental effects such as, for instance, employment repercussions, economic multipliers, potential effects on the related industries, economic and environmental sustainability, impact on the landscape. Finally, in order to take into consideration, the time value of the money, we have to adopt as discount rate the marginal production opportunity cost for private entrepreneurs, or the social discount rate for public investments.

3.2. LCC: Life Cycle Costing

LCC is a type of analysis that can be applied in various construction circumstances: for a single complete plant, for a set of components or a single component, to support decision-makers too. This analysis can be used for an existing activity as a method for evaluating future operating budgets, or for evaluating improvement options. The period that used for the analysis should be the entire life cycle of a constructed asset. In order to apply the methodology, the main features of each project should be already well defined. This methodology can improve the transparency of cost composition and decision-making process, supporting in more effective way the achieving the desired objectives.

Thanks to the LCC approach, the overall cost of a project can be determined, including the costs of planning, design, purchase, use, management, maintenance, disposal. Finally, it is used for the financial evaluation of alternative solutions identified in the course of a sustainability analysis (Clasadonte and Matarazzo, 2011).

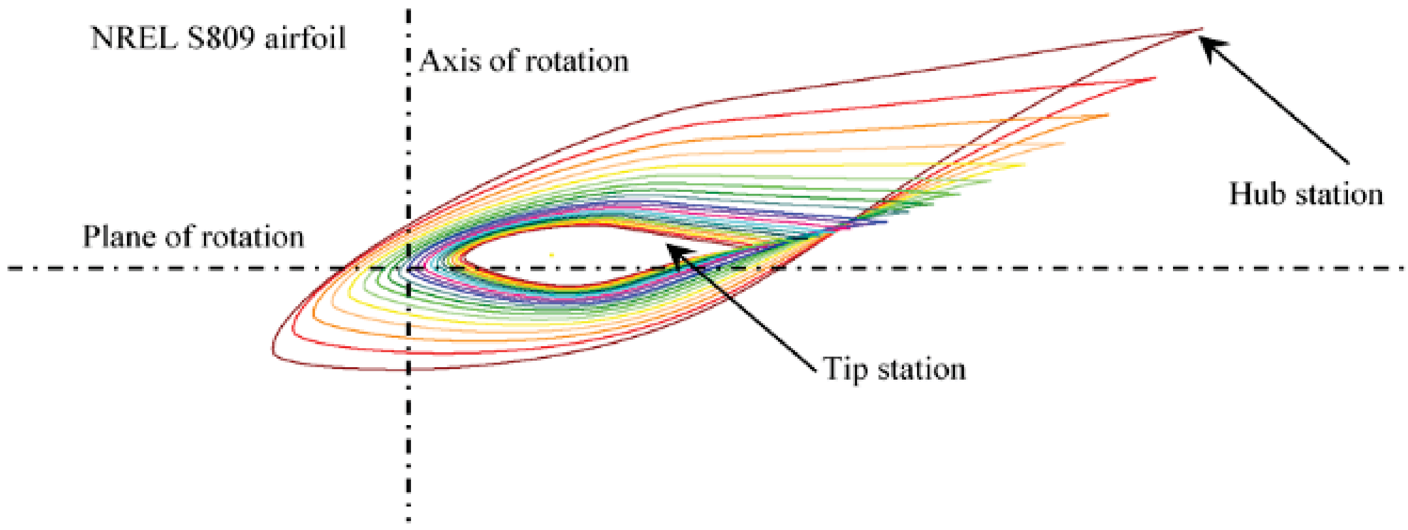

Fig. 7. 2D representation: Taper and twist of the designed wind rotor

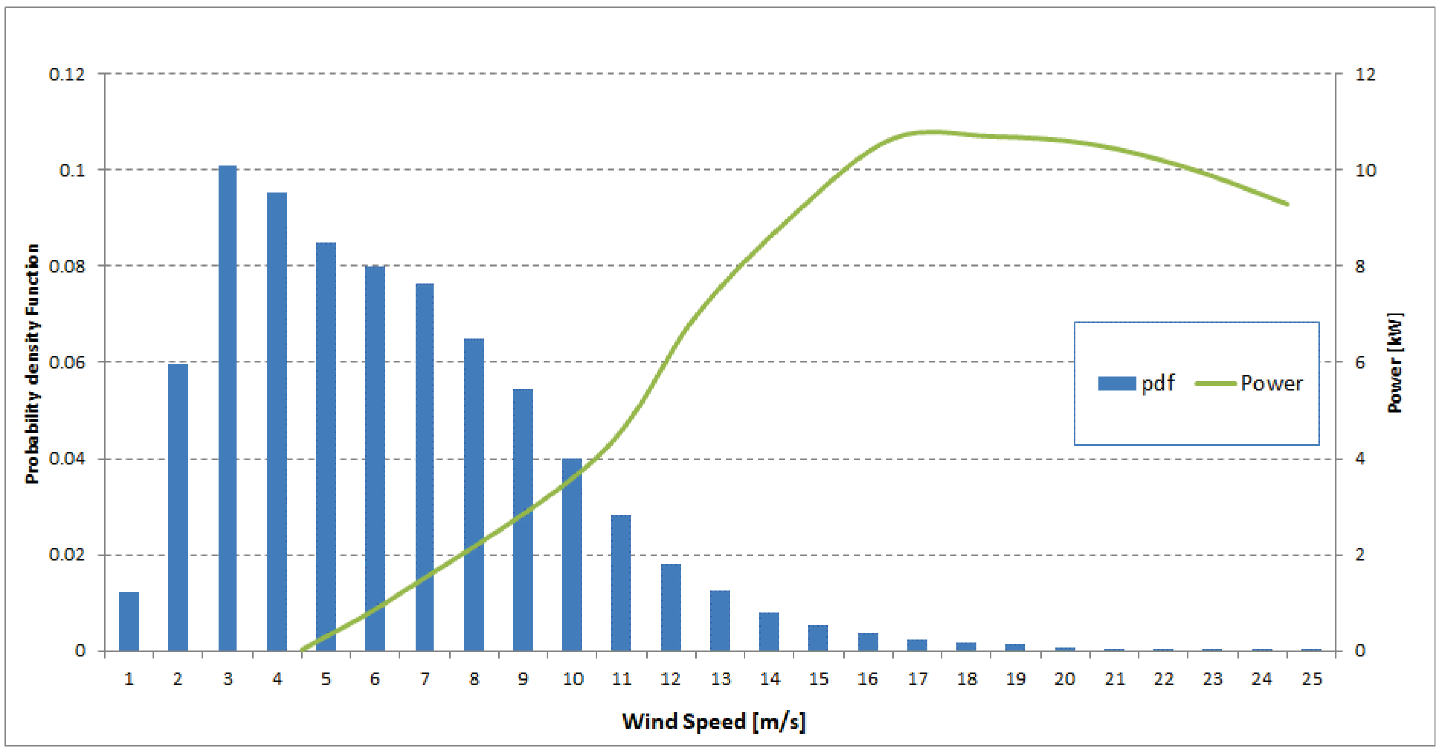

Fig. 8. The final power curves

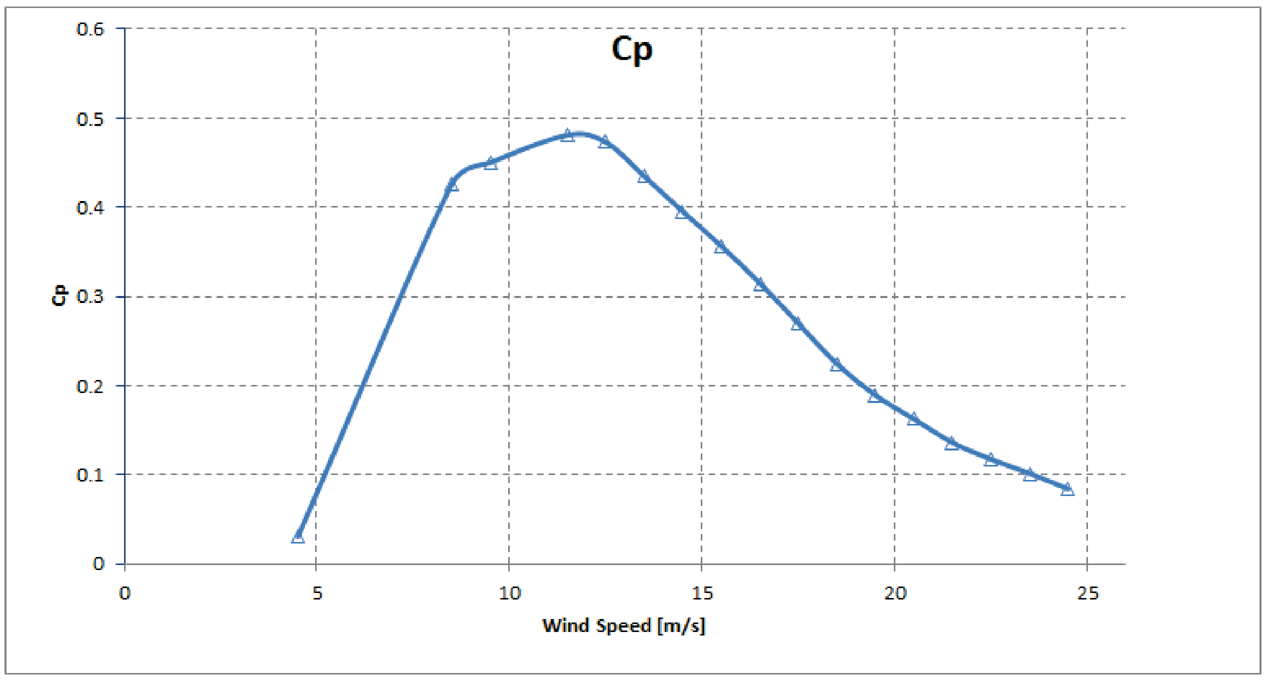

Fig. 9. The final power coefficient curve

LCC is therefore "the tool to support decision-making processes and allocate resources between alternatives of real estate intervention of new construction or renovation", suggesting the most advantageous solution, considering the performance and a time frame equal to the life cycle of the building. The methodology leads to the formulation of more verified solutions related to actual performance, thus arriving at a single indicator, also called "economic efficiency index".

Through this methodology, different projects, materials and technological solutions are evaluated, thus identifying a different relationship between construction cost, maintenance cost, and computing payback period. As a result, it is possible to observe significant differences in current operating costs and maintenance costs, energy consumption and component replacement cycles (UNI EN ISO 14040; UNI EN ISO 14041; UNI EN ISO 14042: UNI EN ISO 14043).

It is important to stress that a "traditional" LCC is not an environmental accounting tool just because it contains life cycle words (Matarazzo et al., 2018) and it is often used in an environmental context. Hence the need to correlate the two different approaches, certainly obtaining an overall vision based on multiple points of views. Analysing LCA and LCC we can see some differences such as: LCC analysis combines all relevant costs for making investment decisions; LCA analysis analytically measures the different possible environmental impacts, based on environmental criteria scores, and the different categories of damage. To date, combining LCA and LCC is a practice that is spreading all over the world as it manages to combine aspects related not only to economic sustainability, but also to environmental sustainability. The application of the joint LCC and LCA provides a solid basis on which to start a rational decision-making process.

4. Conclusions

In this paper a new wind turbine has been proposed for low wind installation site and high-power coefficients.

The optimization of the wind turbine geometry is simple and the methodology is quite original and innovative. It is based on the choice of the design wind speed and the design angle of attack through the use of the Blade Element Momentum Theory.

The final objective is to design a wind turbine able to maximize the Annual Energy Production in low wind installation sites.

In conclusion, it can be said that technical solutions to improve energy efficiency exist, able also to reduce environmental impacts. Moreover, carrying out suitable financial, economic and environmental analyses, keeping up with technology, private companies will be able to implement them. To this end, it is important to make companies increasingly aware of important issues also with regard to their activities and social responsibilities.

In a future paper, we aim to test the wind turbine in conditions of maximum performance. Additionally, once each cost item has been determined, we will apply the LCC analysis through the use of the SIMAPRO software.

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CIRCULAR ECONOMY GOOD PRACTICES IN WASTE MANAGEMENT AND PREVENTION IN THE FOOD SYSTEM

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Abstract

The food system is one of the most important sectors affecting the transition to a circular economy. Through more efficient use of resources, a circular economy in the food system can contribute to economic growth and climate change mitigation, creating new market opportunities. Food loss, waste and surplus are in fact, related to the inefficient use of resources. All these inefficiencies throughout the various phases of the food system generate impacts not only at the environmental, but also at the societal level.
This paper aims to identify strategies associated to innovative food system good practices that support more efficient food waste prevention and management and the adoption of a circular economy approach. For this purpose, 56 circular economy good practices related to the food system were analysed.
This work is based on studies carried out in Italy in the framework of the Italian Circular Economy Stakeholders Platform referring to European circular economy good practice criteria. An official definition of a circular economy good practice has not yet been worked out, but this study singled out new approaches to classifying and analysing them for future implementation of circular economy standards. Moreover, the analysis made it possible to identify gaps in the food system and the strategic actions needed to close them through a systemic and integrated approach covering the various phases of the food system.

Key words: circular economy, food system, food waste prevention, food waste reduction, good practices

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1. Introduction

According to a recent UN research, about 17% of total food available to consumers in 2019 became waste (UNEP, 2021). Such a large amount of waste in all its various forms (loss, waste, surplus) can be attributed mainly to the enormous complexity of the food system (FAO, 2019; Foran et al., 2014) which includes processes starting from different primary resources, as well as the economic, social and natural environments in which these are embedded (FAO, 2014). The greater its complexity, the greater its environmental impact in terms of resources and greenhouse gas emissions (FAO, 2015). Conversely, foods that require minimal processing, including short-chain products, impact less (Kiss et al., 2019).

Socio-economic conditions have a strong influence on food waste (FAO, 2011). In high-income regions, in fact, waste is greater in the later stages and mainly during consumption. In low-income regions, on the other hand, food waste occurs most often during post-harvest handling, aggregation and storage, and is mainly due to economic problems (FAO, 2013; Parfitt et al., 2010). Food waste is therefore a clear example of inefficient use of resources with causes differing greatly depending on the phase in which they are produced (Göbel et al., 2015). Impacts affect not only

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the environment but also, dramatically, society (Seberini, 2020).

Hence, preventing and reducing food waste requires actions during all phases of the food system, with different strategies depending on the specificities of the individual phases and the production and consumption contexts. Such an approach finds expression in the circular economy (CE) perspective, which includes waste management and prevention strategies (European Parliament, 2015; EMF, 2013). According to EU programmes (EC Communication 2020a; EC Communication 2020b), the CE provides a systemic approach to transforming waste into resources and addressing the food system comprehensively.

In Italy, food waste prevention strategies and actions were introduced by the so called "Gadda law" (GD, 2016) which contains provisions concerning "the donation and distribution of food and pharmaceutical products for the purposes of social solidarity and the limitation of waste". This law, which regulates existing norms on tax concessions, civil liabilities and procedures for hygienic-sanitary safety, introduced advantages for those who donate their surpluses (as opposed to destroying them), such as reductions in garbage tax and facilitation of administrative proceedings for donation procedures. Yet, it also promotes the recovery of food for human consumption (to avoid destruction) as a value of and the creation of a Coordination Table within the Ministry of Agriculture, Food and Forestry Policies for consultation among all those involved to counter food waste and poverty. Thanks to this law, the recovery and redistribution of food surpluses for social purposes is fostering the transition towards a circular economy while improving collaboration between food supply chain stakeholders.

In order to identify and develop effective strategies for reducing food waste, a systemic and integrated approach has to be implemented, keeping the specificities of the phases of the food system and the contingent socio-economic systems in mind. To this end, the paper aims to explore the association between 56 food waste prevention actions carried out in Italy and the circular economy pillars set down for controlling food waste.

The linkage between circular economy good practices (CEGPs) and waste prevention has been explored by Cappellaro et al. (2020) through an analysis of more than 30 CEGPs in one Italian region (Emilia-Romagna), that was a first attempt at establishing criteria for the identification of CEGPs. In fact, there are still no precise criteria for the identification of CEGP. Actually, a Technical Committee on the Circular Economy was recently established in the framework of the International Standard Organisation (ISO) with the aim of developing "frameworks, guidelines, supporting tools and requirements for the implementation of activities of all involved organizations to maximize the contribution to Sustainable Development" (ISO/TC323, 2021). Similarly in Italy, the National Unification Authority (UNI) has set up a Technical Committee on the Circular Economy (UNI/CT057, 2021), which has however not yet published a standard, only some working documents.

A reference and representative criteria method for CEGP collection was recognised in the European Circular Economy Stakeholder Platform (ECESP, 2018; Cappellaro et al., 2020). The ECESP was created in 2017 by the European Economic and Social Committee (EESC) and the European Commission (EC) with it's the aim, among others, to facilitate the exchange and mapping of national, regional and local circular economy good practices, as well as examples from businesses, trade unions and civil society organizations. The Italian Circular Economy Stakeholder Platform (ICESP) is the Italian mirror initiative and one of its aims is to stimulate the collection of good circular economy practices in Italy. In 2020, more than 80 good practices were collected in the ICEGP database on the basis of ECESP criteria. ICESP outputs are also present in the ECESP, thereby introducing Italian results in Europe and contributing to the European Circular Economy Agenda. The key factors for potential transferability are based on the relationship between the Italian and European platforms, a feature that makes the model perfectly transferred to other member countries.

On the basis of these considerations, this study carried out an analysis of 56 CEGPs collected according to ECESP/ICESP.In particular, the research approach deals with the following phases:

- collection of food system CEGPs;
- classification of food system CEGPs according to the food system phases and circularity pillars;
- analysis of CEGPs frequency distribution in the food system phases and in the circularity pillars;
- identification of associations among food system phases and circularity pillars.

2. Material and methods

2.1. Collection of food system Circular Economy Good Practices

According to the ECESP (2018), "Good practices are relevant initiatives, innovative processes and 'learning from experience' examples involving companies or other relevant stakeholders such as research, academia and civil society". The circular economy good practices (CEGPs) considered in this paper were evaluated on the basis of ICESP (Italian Circular Economy Stakeholder Platform) criteria, which are similar to those of ECESP (European Circular Economy Stakeholder Platform), however the criteria of replicability was also added (Cappellaro et al., 2020).

Fifty-six CEGPs related to the Italian food system were collected in the period January-May 2020 on the basis of a study reported by the ICESP working groups on "Sustainable and circular design, production, distribution and consumption systems"

(ICESP, 2020) and "City and Territory" (ICESP, 2019).

2.2 Analysis and classification of food system Circular Economy Good Practices

The authors then classified the CEGPs found in the ICESP studies according to the food system phases in which they occur and the circular economy pillars they implement. This classification required a new definition of the state of the art of food system phases, which had to be formulated in accordance with a circular economy approach. In particular, each CEGP was associated only to the circularity pillar in which it is implemented the most. The list of CEGPs is included in the supplementary material.

2.2.1. Food system phases

To understand the importance and severity of the food waste phenomenon, circular economy good practices (CEGPs) have to refer to the whole food system not just the value chain. The value chain merely involves the profit at each stage, while the whole food system provides a wider and clearer view of each phase from primary production to consumption and post-consumption.

In the literature, food system phases differ depending on the classification method and whether it focuses more or less narrowly on production (primary and transformation) phases (FAO, 2011; Humphrey and Memedovic, 2006; TEEB, 2020). However, since food waste does not occur only in these phases, an agri-food system including the management of surpluses, among other things, is more appropriate.

During primary production, for example, losses are generated by the incorrect timing of harvesting, inadequate harvesting and handling, inappropriate trading and climatic conditions. During post-production, significant losses are caused by inadequate storage and conservation conditions. In the processing industry, food losses and waste depend mainly on the processing efficiencies of the various stages, which vary greatly depending on the product. Overstocking, packaging, accidental damage and technical malfunctions can generate transformation losses. The post-sale phase can also produce waste, for example during catering and at home due to a lack of knowledge of daily food management and label consciousness. Table 1 gives examples of food system phase definitions cited in literature.

To improve the description of the system, other key ECESP Circular Economy areas for CEGPs were taken into consideration, such as production, consumption, secondary raw materials, waste management, and innovation and investment (ECESP, 2018). Therefore, according to the authors, the food system can be represented by the following phases in each of which waste is generated (in grey in Table 1).

• *Agricultural production* including post-harvest, handling and storage, where losses are due to mechanical damage and/or spillage, the sorting of crops, and degradation during handling, storage and transportation between farm and distribution;

• *Processing* where losses are mainly due to sorting, washing, peeling, slicing and boiling, as well as process interruptions, accidental spillage and degradation;

• *Distribution, marketing and retail* generate losses related to logistics such as incorrect stock management, meeting product quality expectations, and inefficient organization between sectors resulting in overproduction, mishaps, and/or damage;

• *Consumption* leads to waste caused by food badly cooked, not well preserved and/or not used before the expiry date. At this stage, waste is generated by a lack of awareness and ability to manage the food;

• *Secondary materials* imply the use of some agro-industrial by-products in a circular approach, as innovative and functional ingredients in value added foods;

• *Waste management* involves interdependent rather than non-alternative actions to reduce the amount of no longer recyclable waste.

Table 1. Definitions of food system phases and food system phases in authors' view (in grey)

References	***Food system phase***						
FAO (2011)			Consumption	Distribution	Processing	Post-harvest handling	Agricultural production
TEEB (2020)			Household consumption	Distribution, marketing, and retail	Manufacturing and processing	Agriculture production	
Humphrey and Memedovic (2006)			Retail		Processing	Production	Breeding and farm equipment companies
Nobili and Cappellaro (2021)	Waste management	Secondary materials	Consumption	Distribution, marketing and retail	Processing	Agricultural production	

According to the authors' analysis, these phases were the only ones in which good practices were found to occur; other phases with good practices were detected.

2.2.2. Circularity pillars

CEGPs were also classified with reference to five circularity pillars which, as reported in Lacy et al. (2016), are strategies that address environmental sustainability while generating opportunities in terms of innovation, competitiveness, job and value creation.

With reference to the food system, the circularity pillars for CEGPs are:

• *Sustainable inputs*, meaning use of renewable energy in the production phases and/or organic food in processing phases (Cerutti et al., 2018);

• *Life extension* relates to strategies to extend the shelf-life of food products (i.e. eco-packaging) (Guillard et al., 2018);

• *Sharing platforms* refer to web platforms for sharing surplus or exchanging by-products within communities or industrial symbiosis platforms (Cutaia et al., 2015; Sposato at al., 2017);

• *Product-as-service* in this case means, for example, ordering food online and having it delivered to one's home (Muñoz López et al., 2020);

• *End of life* means the transformation of food waste into compost and/or its valorisation for energy purposes such as biogas (Aliasgari et al., 2019).

3. Results and discussion

On the basis of the foregoing criteria, the CEGPs analysed fell into more or less all the food system phases (Fig. 1) and systematically implemented circularity pillars. In particular, the frequency distribution of the collected CEGPs refers, to varying extents, to food system phases described below:

1. *Agricultural production:* CEGPs are related to innovative agronomic practices such as the use of biodegradable mulch films and microorganism consortia to promote plant growth;

2. *Processing:* CEGPs involve innovative farming modules and hydroponic vegetable cultivation;

3. *Distribution, marketing and retail:* CEGPs refer to environmental quality labels and the digitalisation of the supply chain;

4. *Consumption and post consumption:* food surpluses are collected and distributed to people in need. This activity requires efficient logistical organisation to make the times and costs of collecting and distributing meals economically sustainable. Other CEGPs related to this phase relate to the use of compostable tableware;

5. *Secondary materials:* CEGPs illustrate the valorisation of agri-food by-products as a source of valuable bioactive compounds for producing new materials (textile fibres, packaging, food; building and biomaterials);

6. *Waste management:* CEGPs relate mainly to the regulation of separate waste collection and the conversion of waste for energy purposes.

Quantitatively, the analysis showed that the phases most frequently represented were, equally: "consumption and post consumption", "secondary materials" and "waste management". Instead, only a few CEGPs were related to "agricultural production", "processing" and "distribution". In particular, the new strategies that emerged for food waste management and prevention in accordance with a circular economy approach promote:

• innovation in agronomic practices to make agriculture more sustainable;

• designing production so that it is more sustainable and circular, using waste from other productions;

• establishing criteria, methods and applications that develop an approach to waste prevention and raise the awareness of industrial and (hotel, restaurant and café - ho.re.ca.) operators;

• bringing about changes in culture and behaviour, by raising consumer awareness of purchases and consumption through the dissemination of information and events, and the adoption of new urban models of circular communities (co-housing, collective purchases, short supply chains from organic agriculture, to fair trade, etc.);

• the use of by-products in a circular approach often promoting industrial symbiosis for the health and well-being of consumers and the environment;

• communicating actions, including information on the specifications and innovations of the services, and teaching the public about the correct separation and disposal of waste and the potential of wet waste compost and biogas.

Classifying CEGPs according to the circularity pillars revealed that the pillar by far most frequently represented is "Sharing, use and consumption", while the least represented were "Product as a service" and "product end of life" (Fig. 2). Looking at the distribution of circularity pillars in CEGPs suggests that the following strategies would create some advantages and make it possible to overcome the unsustainability of the current food system:

• sharing platforms optimise food system costs and favour resource-efficient use in consumption phases

• sustainable inputs reduce the environmental footprint of food systems

• life extension prevents food waste.

• product-as-a-service significantly reduces environmental impact and fosters innovation in the distribution, marketing and retail phases

• extending products' end-of-life improves the sustainability of waste management phases.

The evaluation of good practices with respect to both phases and pillars, which may suggest further strategic actions for the management and prevention of food waste within the food system, can be summarized as given in Table 2.

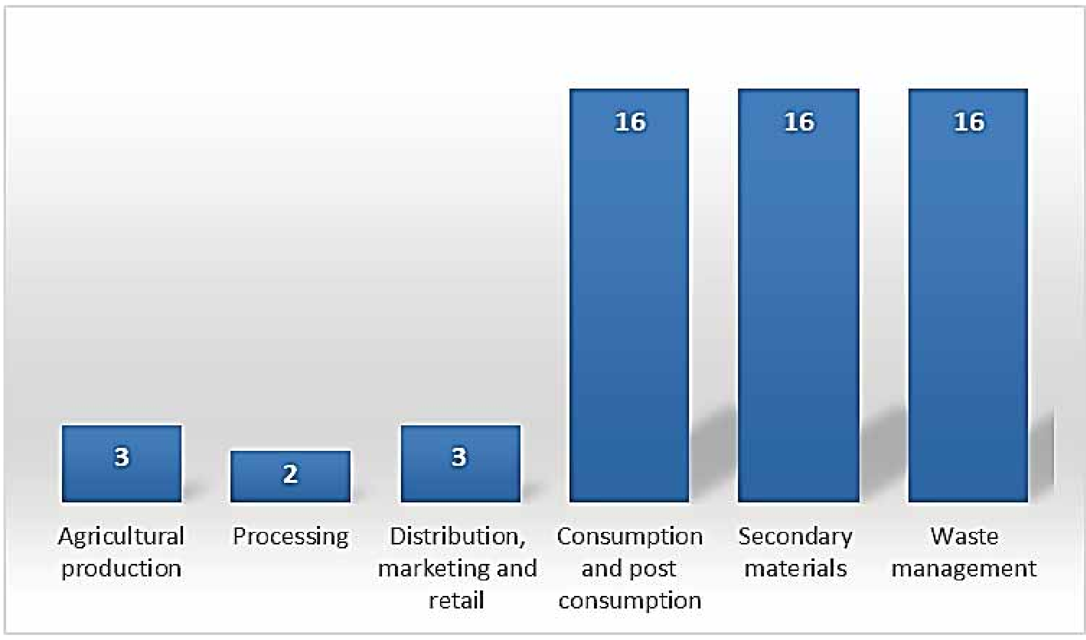

Fig. 1. Frequency distribution of CEGPs in food system phases

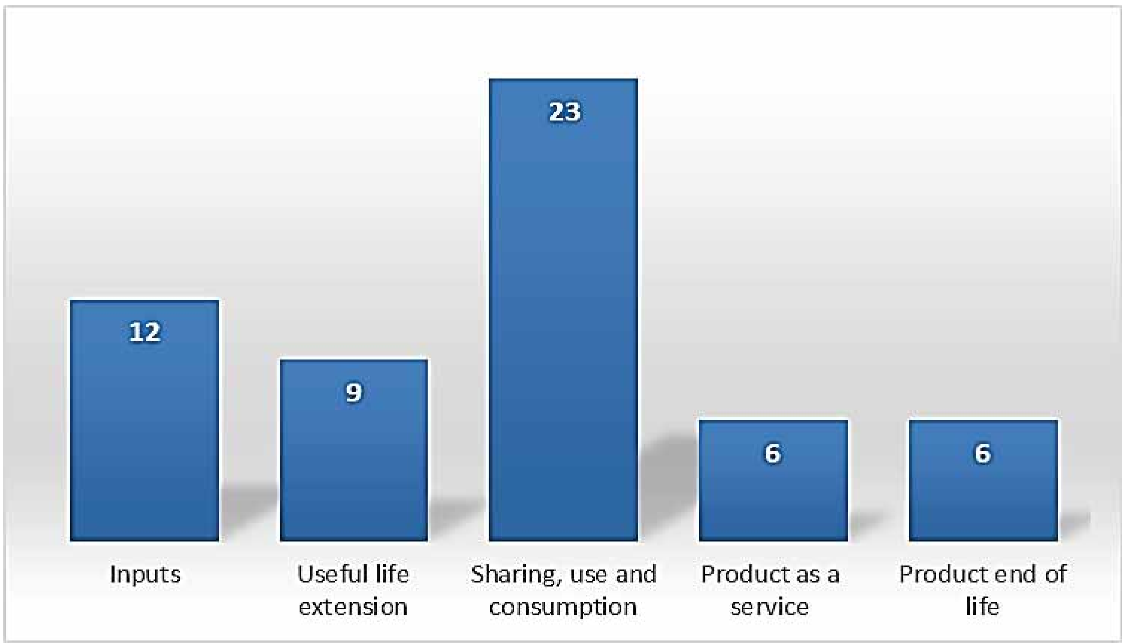

Fig. 2. Frequency of the distribution of CEGPs in the circularity pillars

Figures displayed in the "circularity pillars" Table refer to the CEGPs listed in the supplementary material. Each CEGP was considered only once in Table 2 depending on the main pillar it implements. The Table shows that the most frequent associations include surplus distribution to optimise food system costs and resource-efficient use in consumption phases; the use of agri-food by-products as innovative value-added ingredients; and new technologies and materials for preventing and reducing crop losses as inputs for primary production.

The first association points out that synergies established between different users reduce the production of waste; improve its quality, collection, transformation and reuse; and monitor actions relating to the quality and quantity of the organic residue collected (Saha et al., 2010). As described in the Introductory paragraph, this approach, particularly in Italy, is encouraged by the so called "Gadda law" (GD, 2016).

The second association, related to the use of by-products, is in line with what is emerging from the third "Italian circular economy report" (Circular Economy Network, 2021). The report points out that Italy is in second place behind France for the circular use of materials (19.3%). The recycling of secondary raw materials is, then, a way to redirect the system towards a circularity perspective that leads to a decrease in the impact (of food waste) and towards climate neutrality. Efforts must be concentrated on the creation of products designed to last longer, especially in a context characterized by intense use in a short period of time or by a second life immediately following the first (Fifield and Medkova, 2016).

Finally, another association concerns new technologies and materials as inputs for agriculture production. Important directions on this issue arise from the new European Farm to Fork paradigms, the new action plan (EC Communication, 2020a) for the circular economy and biodiversity strategy for the agri-food sector. An enormous effort is being made to enhance sustainable agriculture, organic production, agroecology and other innovative management forms allowing for the reduction of the use of pesticides without compromising the fertility and microbial richness of soils so as to guarantee the safety and healthfulness of foods and thereby protect human health. Noteworthy is that the majority of CEGPs analyzed referred to the downstream phases of the food system, contributing to defining strategies aimed at sharing surpluses through web platforms and charity networks or via industrial symbiosis platforms, while fewer CEGPs referred to the upstream phases of the food system.

Table 2. Associations of the different phases of the food system and circularity pillars. Figures represent CEGPs as listed in the supplementary materials

Food waste management and prevention strategies	*Food system phases*	*Circularity pillars*				
		Inputs	*Useful life extension*	*Sharing, use and consumption*	*Product as a service*	*Product end of life*
Technologies and materials for preventing and reducing crop losses through soilless cultivation	Agricultural production	1, 2, 3, 4, 14, 25, 42				
Agreements with wholesale markets and large-scale distributors to limit waste and the rejection of non-uniform products, and promote the sale of products in bulk	Agricultural production, processing, distribution, marketing and retail		6, 9, 12, 55			
Communication and awareness-raising campaigns to change consumers' concepts of the quality of agricultural products; direct sales from farms	Agricultural production, Consumption and post consumption		7			
Communication and awareness-raising campaigns to change consumers' ideas of food value and the need to reduce food waste in the family, company canteens and at the catering level	Consumption and post consumption, Waste management		11, 13, 38			
Communication and awareness-raising campaigns to bring about a cultural change in consumers about conscious purchases, short supply chains, and local e-commerce	Distribution, marketing and retail, Consumption and post consumption, Waste management		10			
Creation of circular communities for collective food purchases through purchasing groups	Distribution, marketing and retail, Consumption and post consumption, Waste management			8		
Linkage between places where food surpluses originate (company and school canteens, neighbourhood markets, food stores, events) and charity associations for the needy	Distribution, marketing and retail Consumption and post consumption,			15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25		
Treatment of inedible food waste for producing compost and biogas	Waste management				29, 33, 41, 43, 53, 54	
Treatments of inedible food waste for producing secondary materials	Processing, Waste management					45
Systems to optimize the collection of organic waste for compost and biogas production (e.g. use of compostable tableware in collective catering, use of bioplastic bags in neighbourhood and wholesale markets)	Waste management					34, 35, 26, 36, 37
Valorisation of agri-food by-products by extracting valuable bioactive compounds	Processing, Secondary materials			39, 40, 49, 52		
Use of agri-food by-products for producing new materials (textiles fibres, packaging, wasted bread medium paper; building materials; biomaterials)	Processing, Secondary materials			5, 27, 31, 46, 47, 48, 50		
Secondary materials for producing new products	Processing, Waste management	30, 32, 44, 51, 56				

To fill this gap, the development of additional GPs concerning the upstream phases of the system (i.e. primary agriculture production, processing and distribution) must be encouraged. Some proposals along these lines emerged in the working groups studies of the ICESP platform:

- soil care, that is rethinking the economic system involving land in an integrated way, taking the opportunity to transform soil vulnerability into a driving force for a truly sustainable recovery through the promotion of agro-ecological infrastructures;
- digitalization of the agri-food chain from primary production to the processing industry, as well as logistics in favor of product traceability;
- design and development of new technologies, including new forms of eco-packaging, that increase the shelf-life of food, thus reducing waste and improving the sustainability of agri-food production.

Future perspectives for making food products compliant with the principles of circularity and resource-efficiency have been provided by the European Commission, which has proposed measures that will expand the Ecodesign Directive. This approach is even more important since up to 80 percent of the environmental impact of products is determined in the design phase (EC Communication, 2020a), Ecological redesign of the food system starting from the early phases will favour sustainability, which has to take into consideration socio-economic aspects, especially in the current context to support the food and nutritional needs of a growing and increasingly urbanized population

4. Conclusions

The central role of food not only for our survival but in many other areas of personal and public life is widely recognised. Indeed, food plays an important role in economic, ecological, social and political terms. It is of essential value for human health, well-being and prosperity. Yet, the waste produced by the current food system is an enormous problem, considering that every year around 1.3 tons of food are not consumed worldwide, while a billion people suffer from and millions die of hunger. For years, efforts have been made to tackle the problem in its various aspects, so that a large number of good practices related to reducing food waste and losses in every phase of the food system, from primary production to consumption, have been identified.

In this study, 56 circular economy good practices, considered in relation to food system phases and circularity pillars, were collected from the ICESP platform, established much like the ECESP and representative at Italian level of a large variety of circular economy stakeholders from public institutions, firms and industry associations, universities and research organizations, citizens and third sector. Moreover, based on agreements between ICESP and the corresponding European platform (ECESP), the CEGPs collected by ICESP are being evaluated for inclusion in the ECESP database. Consequently, CEGPs are not only relevant nationally, but can also be taken as a reference in a European context.

The CEGPs collection and classification method used in this study was based on ICESP/ECESP criteria and can be seen as a first attempt to identify universal criteria that can be used for the implementation of international standards such as ISO or UNI.

The selection and analysis methodology of circular economy good practices carried out in this paper has made it possible to identify the gaps in the Italian food system and propose strategic actions to implement new circular approaches to controlling food waste in all the food system phases.

In particular, this study has confirmed that CEGPs can provide important examples for managing and preventing waste. Nevertheless, it appears that most of the Italian good practices currently refer to the downstream phases of the food system, in association with circularity strategies aimed at reducing food waste and relating mainly to the sharing of food surpluses with needy people and reusing and enhancing by-products for consideration as second raw materials. As a final consideration, more work needs to be done on prevention in the upstream phases of the food system supply chain. This could be favoured by policies and action plans (EC Communication, 2020a) promoting the adoption of eco-innovation in soil care and throughout the agri-food chain in accordance with life cycle thinking.

Finally, the introduction in the food system of eco-design strategies could drive food waste reduction and ensure that prevention progressively become the norm throughout the food system phases.

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https://www.icesp.it/sites/default/files/DocsGdL/L%27economia%20circolare%20nelle%20filiere%20industriali%20i%20casi%20Costruzione%26Demolizione%20e%20Agrifood.pdf.

Appendix

Table 3. CEGPs analyzed in the paper. The CEGPs are available for consultation in Italian language on https://www.icesp.it/buone-pratiche and in ICESP, (2020) at the following web site: https://www.icesp.it/sites/default/files/DocsGdL/L%27economia%20circolare%20nelle%20filiere%20industriali%20i%20casi%20Costruzione%26Demolizione%20e%20Agrifood.pdf

No	GP TITLE	TOPIC	FOOD SYSTEM PHASE	CIRCULARITY PILLAR
1	NOVAMONT/ MATERBI MULCH FILMS	Biodegradable mulch films for agricultural production	Agricultural production	Inputs
2	RHIZOSPHERIC INTERACTIONS	Agronomic practices for the reduction of external inputs in organic horticulture	Agricultural production	Inputs
3	BIOFECTOR/ SUPRAHUMIC	Composted agricultural waste with and without selected microorganisms as soil conditioner	Agricultural production	Inputs
4	FRESHGURU GREEN HOUSE	Hydroponic cultivation for fruit and vegetable production	Processing	Inputs
5	EDIZERO	Conversion of surplus and recovered materials into high-tech biomaterial	Secondary materials	Sharing, use and consumption
6	BRESCIA MUNICIPALITY AGREEMENT	Conventions and / or agreements with large retailers for the reduction of food waste and packaging	Distribution, marketing and retail	Useful life extension
7	LA POLVERIERA	Urban regeneration project	Consumption and post consumption	Useful life extension
8	SOLIDARIA	Solidarity co-housing	Consumption and post consumption	Sharing, use and consumption
9	RISTORAZIONE SOSTENIBILE 360	Sustainable catering	Waste management	Useful life extension
10	BISOS	Responsible tourism	Consumption and post consumption	Useful life extension
11	PACCOZERO	Communication and awareness-raising campaign	Consumption and post consumption	Useful life extension
12	TRENTO ECO PROVINCIA	Local authority environmental quality branding	Distribution, marketing and retail	Useful life extension
13	LIFE FOSTER	Training, education and communication to reduce food waste in the food service industry	Distribution, marketing and retail	Useful life extension
14	COLTIVARE INLANA	Wool for soilless cultivation	Processing	Inputs
15	AVANZI POPOLO PROJECT	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
16	CIBOAMICO	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
17	POPP PROJECT	Waste management	Waste management	Sharing, use and consumption
18	LASTMINUTE MARKET	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
19	MAGAZZINI SOCIALI	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
20	FOOD BUSTERS	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
21	SIR EMILIA-ROMAGNA	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
22	DISCO SOUPE FIRENZE	Communication and awareness raising campaigns	Consumption and post consumption	Sharing, use and consumption
23	LADISPOLI NONSPRECA	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
24	FONDAZIONE BANCO ALIMENTARE	Food surplus sharing	Consumption and post consumption	Sharing, use and consumption
25	BANCOBUILDING, BANCO INFORMATICO, BANCO FARMACEUTICO	Surplus sharing	Consumption and post consumption	Sharing, use and consumption
26	TORINO CITY LAB	Food surplus sharing	Consumption and post consumption	Product end of life
27	VALLE FIORITA PROJECT	Valorisation of wasted bread as by-products	Secondary materials	Sharing, use and consumption
28	BIOINAGRO	Valorisation of by-products	Secondary materials	Inputs
29	FATTORIA DELLA PIANA	Valorisation of dairy by-products	Waste management	Product as a service
30	FUNGHI ESPRESSO	Valorisation of cafè as by-products	Secondary materials	Inputs
31	CARTACRUSCA	Valorisation of straw as by-products	Secondary materials	Sharing, use and consumption
32	PRESPAGLIA	Primary production by-product reuse	Secondary materials	Inputs
33	PROGEVA S.R.L.	Non-hazardous organic waste recycling	Waste management	Product as a service

34	NOVAMONT AMSA	Eco-friendly separate waste collection in Milan	Waste management	Product end of life
35	NOVAMONT MATERBI	Compostable tableware for better management of organic waste	Waste management	Product end of life
36	NOVAMONT COMPOST	Use of compost from organic waste	Waste management	Product end of life
37	LES OASIS DE EL OIDANE	Composting site creation	Waste management	Product end of life
38	URBANWINS	Communication and awareness raising campaigns	Consumption and post consumption	Useful life extension
39	ENEA-SVILUPPUMBRIA	Added value biomolecule production from agro-industrial waste	Secondary materials	Sharing, use and consumption
40	VALORIBIO	Enhancement of organic waste for agricultural biomaterials	Waste management	Sharing, use and consumption
41	LACITTAVERDE	Compost and biofuel from waste	Waste management	Product as a service
42	BIOXPLOSION	Transformation of organic waste and animal waste into organic humus	Waste management	Inputs
43	OLTRECAFÈ	Collection and transformation of coffee grounds into pellets	Waste management	Product as a service
44	RI-DETERSIVO	Transformation of exhausted oils into surfactant for ecological detergents	Secondary materials	Inputs
45	ADRIATICA OLI	Transformation of exhausted oils into new resources	Waste management	Product end of life
46	PIGMENTO NATURALE	Natural dyes made from agricultural and alimentary discards	Secondary materials	Sharing, use and consumption
47	VEGEA	Transformation of biomass and agro-industrial residues into new materials	Secondary materials	Sharing, use and consumption
48	RICE HOUSE	Primary production rice waste transformed into architectural materials	Secondary materials	Sharing, use and consumption
49	LAVANDULA	Valorization of lavender waste as by-product	Secondary materials	Sharing, use and consumption
50	ORANGEFIBER	Transformation of orange processing by-products into textile materials	Secondary materials	Sharing, use and consumption
51	FUNGOBOX	Reuse of coffee grounds as substrate for mushroom cultivation	Secondary materials	Inputs
52	PACKTIN	Valorization of primary production plant waste to obtain value added molecules	Secondary materials	Sharing, use and consumption
53	COMPOST COMMUNITY	Creation of community composting plant	Waste management	Product as a service
54	LIFE DOP - FERTILIZERS	Enhancement of livestock waste to produce renewable energy	Waste management	Product as a service
55	ENABLING	Use of biomass on biobased product sharing platform	Waste management	Useful life extension
56	VENICE UNIVERSITY PROJECT	Clean energy from wine waste	Secondary materials	Inputs

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EFFECT OF COMPOST AGAINST SOIL-BORNE PLANT PATHOGENS AND ITS IMPACT ON RHIZOSPHERE MICROBIOTA

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Abstract

Compost microbiota and microbial activity play a key role in suppressing soil-borne plant pathogens, starting from rhizosphere, The objective of the present work was to summarize results achieved evaluating compost efficacy against soil-borne pathogens such as *Phytophthora capsici* on courgette and *Fusarium oxysporum* on lettuce and tomato, and explain possible relationships among the targeted host/pathogen and the rhizosphere microbiota due to compost applications. Experimental trials were carried out on potted plants (by mixing compost into the potting substrate) and in two infested fields (by transplanting plants previously grown using potting substrate containing compost). Quantitative Polymerase Chain Reaction - qPCR and the next generation amplicon sequencing technologies were applied on rhizosphere samples. Compost suppressed the diseases by 50-70%, compared to the untreated controls. Moreover, a reduction of the abundance of the soil-borne pathogens up to 100 folds was observed in the soils where compost was applied. The abundance of beneficial microorganisms, such as *Bacillus* and *Trichoderma*, was also influenced and a 10-100 folds increase of it was observed in the rhizosphere of plants treated with compost. However, compost application did not affect the microbial diversity observed applying next generation amplicon sequencing. These findings suggest that compost can be used to reduce plant diseases caused by soil-borne pathogens, most probably improving the abundance of beneficial microorganisms and reducing that of pathogens, but not increasing rhizosphere microbial diversity.

Key words: crop protection, compost suppressiveness, microbiome, plant disease

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1. Introduction

Soil-borne pathogens can affect many plants worldwide, causing root and crown rots, pre- and post-emergence damping-off, vascular wilts and other diseases. Compost can be used to control these pathogens, suppressing plant diseases caused by soil-borne pathogens as well as inducing resistance towards them, as well documented by many authors (De Corato, 2020a; Hadar, 2011; Pugliese et al., 2015; Termorshuizen et al., 2006).

The mechanisms responsible for plant disease suppressiveness of composts are generally very complex, and both microbial activity and microbiota play a major role in the suppression of soil-borne plant pathogens, as Hoitink and Fahy (1986) suggested. Moreover, it has been demonstrated that microbial antagonists are present in suppressive composts and can be isolated from them (Chen et al., 1988; Boulter et al., 2002; De Corato, 2020a; Pugliese et al., 2008).

Many studies have focused on compost suppressiveness of soil-borne diseases caused by *Phytophthora* and *Pythium* species, linking it to the competition for carbon sources and directly to microbial populations and activities (Noble and Coventry, 2005).

In other cases, *Fusarium* wilts are enhanced by the application of composts with higher nitrogen or ammonium content (Hoitink et al., 2001). However, chemical, physical and biological composition can be very different among composts, and, consequently, the ability of compost to suppress soil-borne diseases affecting crops is changeable and often pathogen-specific (Termorshuizen et al., 2006).

Moreover, phytotoxicity problems due to chemical composition, like pH, E.C. and heavy metals, are very well know (Jimenez and Garcia, 1989) and can negatively influence compost applications, in particular for flowers, vegetable and ornamental crops in potting mixes, nurseries and greenhouses. Spermosphere- and rhizosphere-associated microbial communities influence disease development on different plant genotypes (Mazzola and Gu, 2002).

Several advancements based on use of plant disease-suppressive composts have been reached, including novel strategies for the production and application of on-farm compost as well as of compost-based tea (De Corato, 2020a; 2020b). However, a more detailed understanding of the changes occurring for the microbial communities after the application of compost still requires further researches.

The objective of the present work was to summarize results achieved evaluating compost efficacy against the soil-borne pathogens *Phytophthora capsici,* causing Phytophthora blight on courgette, and *Fusarium oxysporum,* causing Fusarium wilt on lettuce and tomato. Another objective was to explain possible relationships among the targeted host/pathogen and the rhizosphere microbiota due to compost application.

2. Material and methods

2.1. Experimental trials on potted plants

In a first set of trials, two different composts were used: (i) a green waste compost (GC), produced starting from green wastes (yard trimming and pruning) composted in a dynamic system for 6 months and sifted with a 10 mm sieve, (ii) the same green compost (GCT), bio-augmented with experimental "*Trichoderma* sp. TW2". The two composts were added at 0, 1, 10 and 20% v/v to a peat substrate (Tecno 2, made with 70% white peat and 30% clay, pH 5.5–6, N 110–190 mg/L, P_2O_5 140–230 mg/L, K_2O 170–280 mg/L, Turco Silvestro terricci, Bastia d'Albenga, SV, Italy) and used for sowing courgette seeds.

One week before sowing, each substrate mixture was infested with 2 g/l of fresh biomass of the soil-borne plant pathogen *Phytophthora capsici* grown in grain-hemp. The fungicide metalaxyl (Ridomil gold, 480 g/l, Syngenta Crop Protection) was applied at the same time as the inoculation and considered as the reference control. Seven days after the infestation with the pathogen, the seedlings were transplanted into pots and placed in a greenhouse on a potting bench.

Each treatment was replicated three times, considering three different pots per treatment and each pot containing 3 plants. A randomized experimental design was applied and the experiment was carried out twice independently. Disease incidence (DI) was evaluated by counting the number of diseased plants in each pot twice during the trials and calculating the percentage of diseased plants.

The fresh biomass of the plants was also weighed. The full description of materials and methods is described in Bellini et al. (2020).

2.2. Experimental trials on field crops

The experiments were carried out under field conditions in Northern Italy on a commercial farm in Moretta (44°45′49.75″N 7°32′29.18″E) as well as on an experimental farm in Carmagnola (44°88′55.188″N 7°68′37.457″E).

The field trials were carried out over two consecutive years, during 2016 and 2017, with the aim to evaluate the efficacy of pre-planting soil treatments against *P. capsici*, *Fusarium oxysporum* f. sp. *lactucae* and *Fusarium oxysporum* f. sp. *lycopersici* starting from the nursery. The two composts previously described were applied at 8 g/seedling at sowing and at 1kg/m^3 of soil before transplanting.

An untreated control was used, while chemical fungicides were applied as a reference chemical control by soil drenching before planting. Disease incidence and severity were scored monthly after transplanting by visually estimation. The full details of materials and methods are described in Cucu et al. (2019), Cucu et al. (2020a) and Cucu et al. (2020b).

2.3. Microbial community analysis

The influence of the treatments with compost on microbial communities was studied at the rhizosphere level by collecting samples from experimental sites at the end of each trials. DNA was extracted and quantitative Polymerase Chain Reaction (qPCR) and the next generation amplicon sequencing (NGS) technologies were applied to study the effects of compost on the rhizosphere microbiota.

The full details of materials and methods are described in Bellini et al. (2020), Cucu et al. (2019), Cucu et al. (2020a), Cucu et al. (2020b).

3. Results and discussion

3.1. Compost suppressiveness

Among the different combinations tested in pots, only the green compost enriched with *Trichoderma* (GCT) applied at 10% was able to significantly reduce the incidence of *Phytophthora capsici* on courgette (Fig. 1).

Regarding the field experimental trials, the results are summarized in Table 1. Composts suppressed the diseases by 50-70% compared to the untreated controls and in a way similar to the application of chemical fungicides.

3.2. Microbial diversity and composition

The results are summarized in Table 2. The abundance of the pathogens (*Phytophthora capsici, Fusarium oxysporum* ff. spp. *lactucae* and *lycopersici*) was always reduced (up to 100 folds) in the compost treated soils in comparison to the other soils. For example, *Phytophthora capsici* passed from an average of 7.24 Ypt gene log copy g/dw^{-1} in untreated control to 5.37 in plants treated with compost (Cucu et al., 2020b).

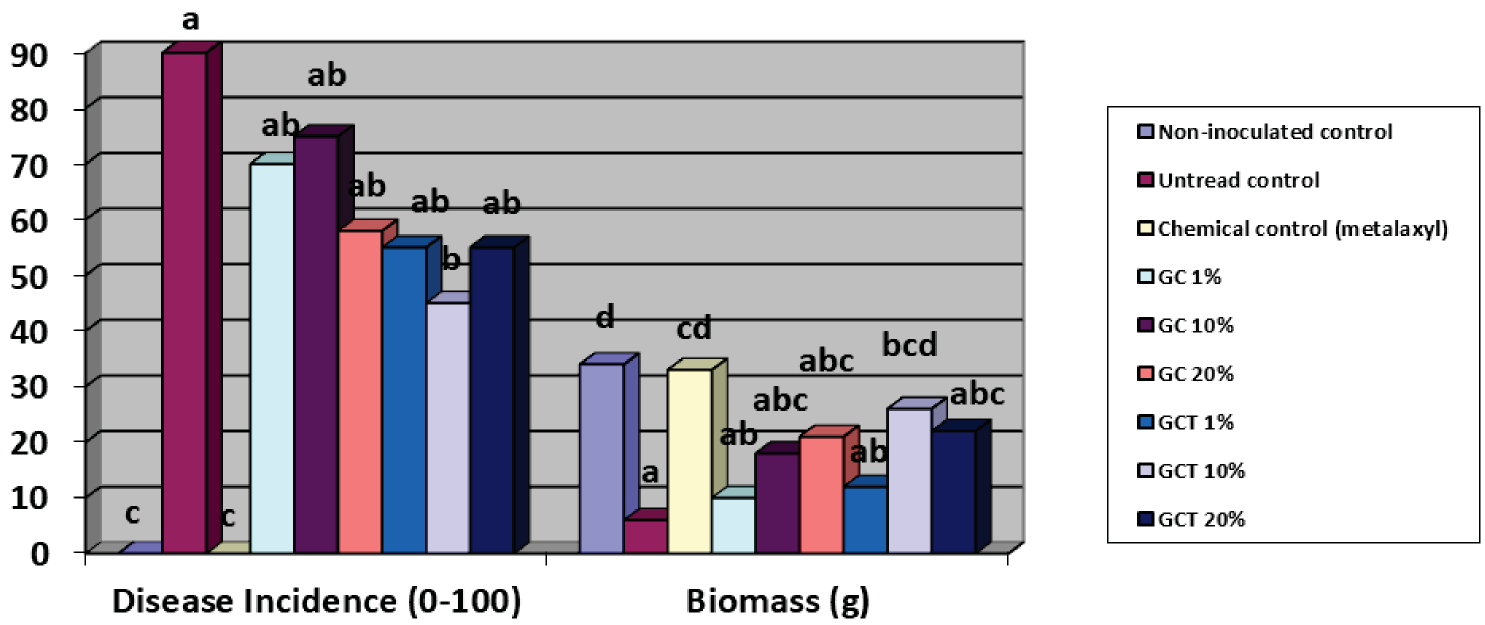

Fig. 1. Efficacy of the compost mixtures to control the soil-borne pathogen *Phytophthora capsici* on courgette plants expressed as disease incidence (%) and fresh biomass (g). The letters refer to the Tukey's post hoc test, which was performed after one-way ANOVA ($P < 0.05$) (Adapted from Bellini et al., 2020)

Table 1. Effect of different compost treatments against *Phytophthora capsici* of courgette, Fusarium wilt of lettuce and tomato in field conditions in 2016 and 2017. Different letters above the number values indicate significant differences between treatments (adapted from Cucu et al., 2019; Cucu et al., 2020a; Cucu et al., 2020b).

Treatment	*Fusarium wilt of tomato*		*Fusarium wilt of lettuce*	*Phytophthora rot on courgette*	
	Disease severity % (2016)	*Disease severity % (2017)*	*Disease severity % (2016-2017)*	*Disease severity % (2016)*	*Disease severity % (2017)*
Green compost (GC)	1.9^{a}	14.5^{a}	30.5^{ab}	17.9^{a}	40.0^{ab}
Green compost Trichoderma (GCT)	10.4^{a}	21.9^{a}	19.2^{a}	16.7^{a}	43.3^{ab}
Untreated control	29.7^{b}	39.9^{b}	61.7^{c}	40.4^{b}	78.3^{c}
Chemical control	Not tested		22.3^{ab} (azoxystrobin)	8.8^{a} (metalaxyl)	34.4^{a} (metalaxyl)

Table 2. Effect of different compost treatments on composition and microbial diversity in field conditions in 2016 and 2017, expressed as significantly improved/reduced in rhizosphere compared to the untreated control (Adapted from Cucu et al., 2019; Cucu et al., 2020a; Cucu et al., 2020b)

Treatment	*Fusarium wilt of tomato*				*Fusarium wilt of lettuce*				*Phytophthora rot on courgette*		
	Pathogen abundance	***Bacterial, archeal and fungal abundance***	***Antagonists abundance (Bacillus, Trichoderma)***	***Functional genes abundance (chiA)***	***Pathogen abundance***	***Bacterial, archeal and fungal abundance***	***Antagonists abundance (Bacillus, Pseudomonas, Trichoderma)***	***Functional genes abundance (chiA, phlD, hcnAB)***	***Pathogen abundance***	***Antagonists abundance (Bacillus, Pseudomonas, Trichoderma)***	***Functional genes abundance (chiA)***
Green compost (GC)	Significantly reduced	Significantly improved (archeal); no variations (bacterial); significantly reduced (fungal)	Significantly improved (*Bacillus*, *Trichoderma*)	Significantly improved	Significantly reduced	Significantly improved (bacterial); no variations (archeal, fungal)	Significantly improved (*Bacillus*, *Pseudomonas*, *Trichoderma*)	Significantly improved (chiA, phlD, hcnAB)	Significantly reduced	Significantly improved (Bacillus and Trichoderma)	Significantly improved
Green compost *Trichoderma* (GCT)	Significantly reduced	Significantly improved (bacterial, archeal); no variations (fungal)	Significantly improved (*Bacillus*, *Trichoderma*)	Significantly improved	Significantly reduced	Significantly improved (bacterial, fungal); significantly reduced (archeal)	Significantly improved (*Bacillus*, *Pseudomonas*, *Trichoderma*)	Significantly improved (chiA, phlD, hcnAB)	Significantly reduced	Significantly improved (Bacillus and Trichoderma)	Significantly improved

Furthermore, the abundance of beneficial microorganisms such as *Trichoderma* and *Bacillus* and of functional genes was also increased (up to 10-100 folds) in the rhizosphere of plants treated with compost compared to the untreated plants. For example, in the case of *Phytophthora capsici/*courgette trial, *Trichoderma* passed from an average of 4.94 ITS log copy g/dw^{-1} in untreated control to 7.05 in plants treated with compost, and *Bacillus* passed from an average of 5.23 16S rRNA gene log copy g/dw^{-1} in untreated plants to 6.07 when compost was applied (Cucu et al., 2020b).

The effects of compost on total bacterial, archaeal and fungal populations varied in different ways for each specific target crop and disease. Regarding next generation amplicon sequencing, differences were observed only when comparing soils from different sites, while compost application did not affect the microbial diversity (Cucu et al., 2020 b).

4. Conclusions

The use of two different composts has been effective in reducing *P. capsici, F. oxysporum* f. sp. *lactucae* and f. sp. *lycopersici* abundance and disease severity at two experimental sites in naturally and artificially infested soils.

The results have shown that, in general, the compost-based treatments resulted in an enhancement of the resident *Trichoderma* spp. and *Bacillus* spp. communities from the rhizosphere, which provide beneficial effects on plants and are also responsible in the reduction of the diseases. However, compost application did not affect the microbial diversity according to next generation amplicon sequencing.

The differences in the total microbial community in the rhizosphere highlighted that compost treatments is safe for the rhizosphere non-target microbial communities as well as for the effective control of the soil-borne pathogens.

This summarized overview suggest that compost can be used to reduce plant diseases caused by soil-borne pathogens, most probably modifying the rhizosphere microbiota and microbial activity and in particular by improving the abundance of beneficial microorganisms and reducing that of pathogens, but not by increasing rhizosphere microbial diversity.

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FROM WASTE TO RESOURCE: BIOWAFER PROJECT

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Abstract

Even though the problem of resource depletion of our planet is getting increasingly worse, most of the input of agro-food industry is discarded, causing expensive management and disposal issues. According to the Circular Economy principles, these problems can be faced by giving more value to wastage, turning it into inputs to innovative supply chains: the biorefineries. The BIOWAFER project addresses those issues investigating how agri-food by-products consistently produced in Emilia-Romagna Region (Italy) can be assigned to consecutive biorefinery processes integrated in order to obtain high-added value molecules for cosmetics and pharmaceuticals. Among all food chains considered, tomato, wine and cheese industries were chosen for waste valorisation. In order to overcome the seasonal waste production, a detailed analysis of storage and stabilization of the by-products was performed. *Streptococcus zooepidemicus* was chosen to obtain hyaluronic acid through waste fermentation process. The biorefinery was integrated with waste bioconversion by *Hermetia illucens* larvae followed by sustainable chemical extraction processes of potential antioxidants, lipids and peptides. Finally, the residues of all the above-mentioned phases will be used for pyro-gasification, to obtain biochar and syngas for agronomic and energy purposes respectively, allowing the closure of the supply chains in a circular way. Many other circular approaches are presented in literature, but, in our knowledge, no one use fermentation coupled with larvae rearing for waste reduction and conversion. Despite some challenges in scaling-up the proposed biorefinery, the project aims to overcome a linear production system by making the supply chains increasingly circular.

Key words: agri-food chain, biochar, biorefinery, circular economy, *Hermetia illucens*

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1. Introduction

The continuous population growth will bring the global population to 9 billion in 2050 (PRB, 2000) further increasing the exploitation of planetary resources (up to 100 Gt raw material consumed in 2030) (OECD, 2012). In this scenario, any recovery that prevents a resource from leaving the economic circle can have a positive impact. Therefore, all the organic wastes can be seen as precursors of functional materials, allowing to limit the exploitation of non-renewable raw materials. This possibility also becomes crucial in view of what was proposed in 2015 by the United Nations in the document "Transforming our world: the 2030 Agenda for Sustainable Development" that incorporates the seventeen Sustainable Development Goals (United Nations General Assembly, 2015). The 12th goal aims to guarantee sustainable production and consumption models suggesting to "do more and better with less",

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increasing the benefits in terms of well-being taken from economic activities, reducing the use of resources, degradation and pollution in the entire production cycle, thus improving the quality of life and prosperity of future generations. In this context, biorefinery systems in which biomasses are converted into a wide spectrum of high added-value products, play a key role. One of the major barrier hindering the development of biorefinery based processes is related to the seasonal nature and the annual variability of the biomass supply that may disfavour the use of several types of feedstocks due to logistic problems and economic unsustainability (Giuliano et al., 2016). To date, waste and by-products of the agri-food industry are often considered wastes and treated consequently, increasing production costs and producing impacts on the environment. As reported in the european FUSION final report project (Scherhaufer et al. 2015), an estimation of landifill and inciniration process of food waste produces a global warming potential of 0.76 and 0.05 kg CO_2eq/kg food waste treated, respectively. In the last two decades, interests in the biorefinery concept is increased exponentially as estimated by google scholar number of pubblications per year since the 2000 using the keyword “biorefinery”.

In literature, several examples of food waste biorefinery are presented, aiming the valorization through extraction of high-value molecules or conversion into biomassess (De Corato et al., 2018) (Teigiserova et al., 2019) (Mohan et al., 2016a; 2016b) (Philippini et al., 2020). Among all possible available scenarios, the use of bacteria and algae are the most explored with insect representing a new possible approach in bioconversions of waste into a high lipid and protein content biomass (Rajendran et al., 2018) (Wang et al., 2017a; 2017b). Insects are known to be capable of digest organic waste producing larvae capable of reducing waste at high rates. Among all the insects adopted in these bioconversions, black soldier fly dipters (*Hermetia illucens*), due to their high waste reduction rates (40-60%) (Mentari et al., 2020), rapresent a good candidate for biorefinery purposes. Moreover, black soldier fly are known to be rich in fat (20-40%) (Chia et al., 2020) and proteins (30-45%) (Chia et al., 2020): while proteins (in terms of amminoacid composition) are not affected by the rearing substrate, fat content (in terms of saturated and unsaturated fatty acid composition) instead is higly dependent on the rearing substrate, with high energy content (carbohydrates) affecting the lipid composition, in particular lauric acid (C12) abundance (Spranghers et al., 2017).

BIOWAFER project research is aimed at identifying how to develop an integrated and sustainable biorefinery for the valorisation of waste from agro-industries in the Emilia-Romagna region. Thereby the present paper explores how it is possible obtaining products with high added value, for the cosmetic and pharmaceutical industries considering the waste and the by-products of the agri-food chains as precursors of basic chemicals and functional materials, allowing to limit the exploitation of non-renewable raw materials. In this paper, a discussion about the development of an integrated bio-refinery system is presented trough a case study in which different techniques and residual biomassess have been integrated in order to overcome the limits of traditional bio-refinery plants.

2. Material and methods

To develop an integrated biorefinery, a part of literature review was carried out for both the techniques and the most representative supply chains of the region and their residual biomasses production. The most promising techniques were selected for obtaining molecules with high added value and an attempt was made to implement them by adopting a circular biorefinery approach. An integration of different techniques has been proposed in the case study, in order to maximise the recovery of active substances while reducing the final disposal of residues.

2. 1. Case study

The biowafer case study is presented in Fig.1. Three agri-food farms have been selected in order to provide residual biomasses. Selected residual biomasses, supplied continuously throughout the year, even if dissimilar in different seasons, will be enhanced by adopting a circular approach of biorefinery.

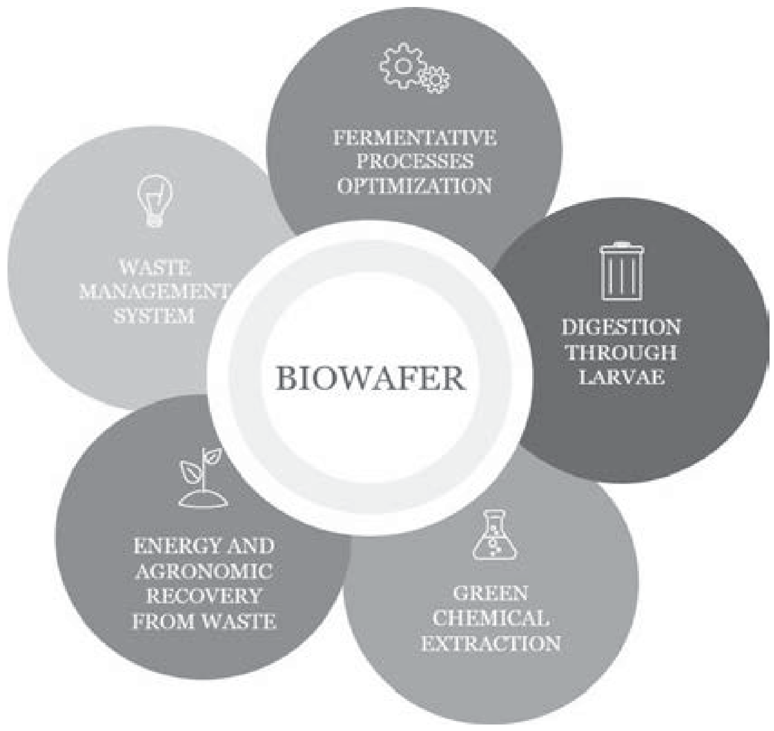

Fig. 1. BIOWAFER project

Through consequential and integrated processes, the input materials of the different phases are enhanced without producing further by-products and waste. Each upstream residue becomes a substrate for the respective downstream phases, and each of the different phases leads to different chemical products with high added value of interest for the cosmetic and pharmaceutical sector.

The techniques used in the biorefinery process include fermentation by selected bacterial strains to obtain hyaluronic acid, polygalacturonans, plant keratin, and lactobionic acid from an adequate mixture of sugars and proteins. The proposed methodology represents an alternative to the extraction of compounds from animal substrates, with significant economic and ethical benefts. Selected by-products will be digested by dipteran larvae, to obtain high added value biomass. In order to maximise the valorisation of by-products, also fermentation residues will be digested by dipteran larvae, to obtain other compounds of interest, including bioactive peptides and polyunsaturated fatty acids. Chemical extraction using conventional and green techniques will allow to extract different molecules, mainly antioxidants. The residues of all the above-mentioned phases will be used for pyro-gasification, to obtain biochar and syngas for agronomic and energy purposes respectively.

The production of energy and the return of biochar as soil improver for agricultural production allow closure of the supply chain in a circular way. In comparison to other circual biorefineries, the use of fermentation coupled with larvae rearing for waste reduction and conversion is a novelty. Despite in this project scaling-up process is not investigated, potential challenges will be taken into account.

2.1.1. Chemical analysis

The residual biomasses have been characterized according the following methodologies (Table 1). For chemical extraction from residual biomasses and from larvae the following methodologies have been used:

– for the extraction of lycopene from tomato peels a solvent ultrasound assisted extraction at 40°C with acetone, ethyl acetate and 2-methyltetrahydrofuran (MTF) has been performed with a liquid solid ratio of 30 mL/g of residue starting from the method reported in (Zuorro, 2020) with some modifications. Lycopene was quantified via a spectrophotometer, reading the absorbance at 503 nm in n-exane;

– for the polyphenol extraction from grape residues a solvent ultrasound assisted extraction at room temperature with ethanol and acetone at different concentration in water was selected considering a solvent/residue ratio of 20 mL/g based on Vatai and coworkers work (Vatai et al., 2008) with some modifications. Polyphenols were quantified via a spectrophotometer, reading at 760 nm using Folin Ciocalteu method;

– moisture of residues was evaluated gravimetrically after incubation at 105°C until a constant weight;

– lipid quantification was carried out in n-exane (or other solvents as indicated in the result and discussion section) gravimetrically after Soxhlet extraction;

– a rapid lipid extraction using MTF was selected for fat recovery from larvae as presented in (Smets et al., 2021). Briefly, 3 g of fresh larvae is mixed with 8 g of MTF and 9 g of bi-distilled water in a centrifuge tube and immersed in a water bath at 45°C for 30 minutes, then centrifuged at 4000 rpm for 15 min in a pre-heated centrifuge. After recovery of the organic phase, other 8 g of solvent are added reaping the extraction steps other 2 times in order to increase the recovery. The extract is then separated from the solvent via a rotary evaporator;

– the characterization of extracted lipids was carried out via a gas-chromatographic method after ester derivatisation in order to observe the main fatty acids profile;

– to extract proteins, one step protein extraction protocol was used. Briefly, defatted insect pellet was treated with 40 mL of 1 M NaOH in water bath at 40 °C for 1 h. The supernatant was neutralized, centrifuged for 15 min at 4000 rpm and then recovered and stored at -20 °C for further uses (Caligiani et al., 2018). Protein content was evaluated via Kjeldhal method for total nitrogen quantification considering 6.25 as a conversion factor. In parallel, bromelain enzyme was used in order to extract protein content. Briefly, defatted insect pellet was treated with 3% bromelain in 0.05 M phosphate buffer pH 8 for 13h at 50 °C followed by a 90 °C treatment in order to deactivate the enzyme. The solution was centrifuged for 15 min at 4000 rpm, the supernatant recovered and stored at -20 °C for further uses (Firmansyah and Yusuf Abduh, 2019);

Table 1. Methods of analysis used for each parameter

Parameters	***Methods***
pH	M.D. agricultural policies 13/09/99 met.III,1 (potentiometric)
Residue at 105°	M.D. agricultural policies 13/09/99 met. II,2 (gravimetric)
TOC	M.D. agricultural policies 13/09/99 met.VII.3 (Walkley)
Nitrogen	M.D. agricultural policies 13/9/99 met.XIV.2 (Kjeldahl)
Fiber	wende U.S. AOAC (15°ED)
Saccharose	UV method
Glucose	UV method
Fructose	UV method
Citric acid	UNI EN 1137 1997
D-lactic acid	UV method
L-lactic acid	UV method
Acetic acid	UV method

– both protein hydrolysates were fractionated in content < 1 kDa, >10 kDa and between these two values and characterized in terms of nitrogen content via Kjeldhal method.

3. Results and discussion

3.1. Selection of the supply chains

The agri-food sector is relevant for the economy of the Emilia-Romagna Region. Given the intensity of local agricultural and agri-food production, the gross specific availability of residual biomasses (mass of dry matter per km^2) is among the highest in Italy (about 80 tons year DM/km^2) (ANPA, 2001).

Emilia Romagna is confirmed as the most productive region in tomato cultivation. Emilia Romagna is the region with the largest proportion of land cultivated with industrial tomatoes, amounting to 25,833 hectares (ISTAT, 2020), which represents almost 68% of the production in the northern area (Emilia Romagna, Veneto, Piemonte and Lombardia) (ISTAT, 2020). The industrial processing of tomatoes generates a significant by-product, of which 10-30% consists of peels and seeds (Beninati et al., 2019). However, the partially dehydrated peels and seeds have a low calorific value. Tomato peels are rich in polyphenol compounds with antioxidant activity, namely carotenes and carotenoids with a protein and lipid content of 13.3% and 6%, respectively (Navarro-González et al., 2011). Among these, the most relevant is lycopene, a molecule known for fruits red-orange typical color.

Lycopene is a liposoluble molecule, mainly known for its antioxidant activity (i.e. biological properties in reducing free radicals) and in protecting the skin from photo-ageing damage; moreover, clinical studies demonstrate a possible correletion as anticancer, antidiabetic, cardioprotective, antinflammatory (Imran et al., 2020). Thus, the recovery of lycopene and other active substances from tomato processing residues is therefore of prime importance, for use in several fields, including pharmaceutical and cosmetic industries.

Moreover, Emilia Romagna produces 6,611,490 hl of wines being the third region for wine production in Italy (ISTAT, 2020). Wine processing residues account for 20% of the dried matter of harvested grapes (Beninati et al., 2019). The reform of the Common Market Organisation in the wine sector entails the progressive reduction, until disappearance, of distillation. It is therefore essential to create a new integrated, sustainable and standardised system which will contribute not only to the problem of disposing of this organic waste, but also to its industrial valorisation. Wine residues are known for being rich in polyphenols, in particular anthocyanins, with high antioxidant properties and as inhibitor for skin ageing (Matos et al. 2019). Like lycopene for tomato peels, anthocyanins also pose some correlation in disease prevention, in particular as anticancer, antidiabetic and ant obesity (Khoo et al., 2017). Thus, the extraction of anthocyanin molecules is of high interest for pharmaceutical and cosmetic industry.

The 11.62% of the Grana Padano PDO cheese (the largest PDO production in Europe), is produced in Emilia Romagna (CLAL, 2021). Whey is one of the main residues of the dairy industry, which produces up to 6 litres per kilo of cheese (PEFCR, 2018). Its traditional use as pig feed is no longer sufficient for the total utilisation of this by-product, and disposal by other means is either expensive or environmentally problematic. One of the most important properties of whey is its high value protein content, known to possess antimicrobial, antihypertensive, antitumor, hypolipidemic, antiviral, antibacterial, and chelating agent activity (Marshall 2004).

Another interesting by-product of dairy sector, in particular for cured cheeses known in the sector as “washed rind”, is the residue of treatment with water, salt and micro-organisms used for ageing the cheese. This residue, indicated as “morge” in France, is not well studied but promising considering hits potential fat and protein content, as well as antimicrobial activity. Fat are well known to be a potential raw material for soaps and creams in cosmetic (Ahmad and Ahsan, 2020), while proteins (and in particular peptides) are largely studied in cosmetology applications for skin and hair treatment (Secchi, 2008).

3.2. Collection, storage, stabilization, chemical-physical characterization of by-products

The seasonality and the amounts available for each supply chain under study is reported in the Table 2 according to the productions of the participating partner companies.

For each residual biomass under study chemical-physical was carried out in order to select, the most suitable storage method . First, standard storage methods were examined and subsequently alternative storage methods were identified: freezing (-20 °C), drying (65 °C) and freeze-drying processes. Other preservation methods based on pH, radiation or addition of chemical agents have not been investigated because no evidence has been found in literature.

The tests were performed in triplicate on all matrices for each parameter. For each parameter the most reliable one has been selected and the corresponding protocol has been defined concerning both the preparation of the sample according to the physical state of the biomass (fresh, frozen, dried, freeze-dried) and the extraction efficiency.

The best stabilization method fro tomato peels is freeze-drying: it allows to maintain the physical characteristics unaltered with respect to freezing and drying (Table 3), and is the most effective also in terms of mass reduction, (about 60%). Freezing and drying are slower processes that deteriorate the product.

Table 2 Annual availability for tomato peels, grape pomace, grape dregs and whey
(Data according to the productions of the partner companies involved in the project)

Residual Biomasses	*Tomato peels*	*Pomace*	*Dregs*	*Whey*	*"Morge"*
Seasonality	August September	September October November	All over of the year	All over of the year	All over of the year
Quantity	1.500 tons/year	15.000 tons/year	3.500 tons/year	40 tons/day	6 kg/day

Table 1 Chemical-physical characteristics of tomato peels in different physical states

Parameters	*U.M.*	*Fresh*	*Freezing 20 °C*	*Drying 65 °C*	*Freeze-dried*
pH		4.46	4.52	4.79	4.69
Residue at 105° C	%	35.41	37.9	94.84	96.52
Nitrogen	N% D.M.	3.02	3.42	0.35	0.27
TOC	% D.M.	56.40	60.22	59.01	63.64
Saccharose	g/kg	2.52	1.03	0.95	2.58
Glucose	g/kg	0.5	0.47	0.10	0.11
Fructose	g/kg	0.12	0.05	0.02	0.14
Citric acid	g/kg	0.14	0.02	0.01	0.15
L-lactic acid	g/kg	1.06	0.61	0.53	1.15
D-lactic acid	g/kg	1.92	0.76	0.70	1.9
Acetic acid	g/kg	2.44	0.84	0.75	2.03
Fiber	% weight	49.32	58.32	52.4	50.22

The pomace, if not used fresh, develops a severe degradation process, so the ideal method of preservation was freezing (Table 4).

Table 2. Chemical-physical characteristics of pomace in different physical states

Parameters	*U.M.*	*Fresh pomace*	*Freezing pomace*
pH		3.67	3.74
Residue at 105° C	%	37.38	36.05
Nitrogen	% N D.M.	0.48	0.3
TOC	%	51.74	51.45
Saccharose	g/kg	0.15	0.18
Glucose	g/kg	0.06	1.58
Fructose	g/kg	0.09	1.73
Citric acid	g/kg	0.07	0.09
L-lactic acid	g/kg	0.12	0.84
D-lactic acid	g/kg	0.04	0.34
Fiber	%	33.47	38.39

The dregs do not require any special care for storage. It can be stored in a container in a dry place, for this reasonfreezing and freeze-drying processes were not applied, The drying method could be effective in keeping the residual biomasses stable over the year (Table 5). Whey can be used fresh or frozen, in fact dry-freezing and drying degrade its chemical characteristics. While the best storage method for "morge" is dry delivery.Results of chemical-physical characterization of whey and "morge" are reported in Table 6-7.

3.3. Optimization of fermentation processes

Potential biotechnological sources for the products of interest were identified and analyzed, in particular focused on: hyaluronic acid and bioactive peptides. Biotechnology has been a tool in food processing and food production for centuries.

Table 3. Chemical-physical characteristics of dregs in different physical states

Parameters	*U.M.*	*Fresh dregs*	*Dry dregs*
pH		3.26	3.53
Residue at 105° C	%	40.23	58.45
Nitrogen	% N D.M.	0.12	0.21
TOC	%	47.72	48.51
Glucose	g/kg	1.82	2.11
Fructose	g/kg	0.53	0.47
Citric acid	g/kg	0.29	0.13
L-lactic acid	g/kg	1.20	0.60
D-lactic acid	g/kg	0.20	0.01
Acetic acid	g/kg	0.10	<0.01
Fiber	% weight	26.39	28.42

Table 4. Chemical-physical characteristics of whey

Parameters	*U.M.*	*Whey*
pH		4.15
Residue at 105° C	%	6.96
Nitrogen	N% D.M.	1.99
TOC	mg/l	32.01
Glucose	g/l	0.29
Lactose	g/l	56.16
Galactose	g/l	1.25
Glycerol	g/l	0.05

Table 7. Chemical-physical characterization of "morge"

Parameters	*U.M.*	*"Morge"*
pH		4.89
Residuo 105°C	%	89.61
azoto	N % D.M.	0.36
TOC	mg/l	52.45
fibra	% peso	2.99

Recently it has become essential in reutilizing food residues from different food supply chains. The exploitation of living organisms, or parts of living organisms, can be a cost-effective solution to the food waste problem. Several examples are available from the conventional biotechnologies, with no need to produce transgenic organisms for improving the processes: a) digestion of residual biomass to obtain biogas; b) fermentation of residual biomass to obtain biofuels, e.g. bioethanol; c) improvement of production of biodiesel or other biofuels from plant biomass; d) biomass used as cheap substrate for production of high-value materials; e) designed fermentation processes to obtain specific high-value chemicals; f) extraction of useful substances from residual biomass.

Hyaluronic acid is one of the possible products with high added value that can be obtained from waste and by-products of the agri-food supply chains. It is a polymer of a subunit composed of D-glucuronic acid and N-acetyl-D-glucosamine (Necas et al., 2008), ranging in weight between 103 to 107 Da. Applications of hyaluronic acid concern medical treatments of joints, eye lubrification, skin texture improvement, tissue reparation and scar formation, nutraceutical products and drug delivery (Fallacara et al., 2018; Huang and Chen, 2019). Being a component of vertebrate tissues, particularly in the extracellular matrix of connective tissues, this substance has been traditionally extracted from animal sources, such as vitreous of bovines or rooster combs. Even though this can be considered a way of reusing animal waste from food supply chains, the process is not sustainable and generates risks for the presence of immunogenic compounds and pathogens. Enzymatic synthesis is possible, with enzymes taken from microorganisms, but it requires high quality reagents.

Bioactive peptides are short aminoacidic chains, from 2 to 40 amino acids in length, which derive from mature proteins through partial proteolysis. Bioactive peptides are among the beneficial features of fermented foods, produced by bacteria, yeasts and fungi, with potential activities as immune system modulators, antioxidants, opioid mimics, cholesterol reduction and antihypertensive action (Pavlicevic et al., 2020). Plant materials from tomato and grape, as well as milk, cheese and whey, contain hundreds of proteins which can be used as starting materials (Maestri et al., 2019).

Growth conditions of strains of microorganisms which can grow on biomass and produce hyaluronic acid (Liu et al., 2011) have been optimized. *Streptococcus zooepidemicus*, is being studied for the possibility of using as a growth substrate residues from the supply chains of industrial tomato, milk and dairy, wine production (Amado et al., 2017). All the selectied residual biomasses containsugars and other molecules which can be substrates for the growth of the bacterium and for the synthesis of hyaluronic acid. The fermentation process is affected by pH, temperature, aeration and stirring, with a moderate stirring favoring the formation of high molecular weight polymers. Interesting possibilities for using plant cell cultures in hyaluronic acid production can also be considered (Rakkhumkaew et al., 2013).

3.4. Waste and by-products digestion by insect larvae

Selected residual biomasses were subjected to digestion through *Hermetia illucens* (Diptera: Stratiomyidae) larvae in order to obtain other interesting compounds for cosmetic and pharmaceutical applications. In the second phase of the project, also residue of the fermentation will be subjected to digestion through *Hermetia illucens* larvae in order to obtain other interesting compounds for cosmetic applications, such as bioactive peptides (Firmansyah and Yusuf Abduh, 2019), polyunsaturated fatty acids - which can be found into the larvae at a percentage of 7% (Smets et al., 2020), and antioxidants peptides (Zhu et al., 2020).

The *Hermetia illucens* larvae used in this study were obtained from the mass rearing of the Department of Sustainable Crop Production (Di.Pro.Ve.S) of the Università Cattolica del Sacro Cuore (Piacenza, Italy).

The rearing was set up in an air-conditioned room (28 ± 2 °C e 50 ± 5% R.H.). In the room, three sections have been set up, each dedicated to a separate development stage of the insect. Adults were reared in a wooden frame holding a mosquito net cage which allowed air and humidity exchange. To provide the required brightness for couplings ($200\ mol \cdot m^2 \cdot s^{-1}$ according to Sheppard et al., 2002), a panel of LED lamp was placed above the cage. The photoperiod was 16 hours of light and 8 hours of darkness. Adults were fed with a solution of water and sugar, placed in a dedicated box. Some supports were placed inside the cage to increase the available area for adult activity and to stimulate their "lekking behaviour", their mating behavior (Tingle et al., 1975). Oviposition took place in the grooves of specific supports, placed in a box also containing decomposing material to attract females. Oviposition supports were replaced every two or three days: supports containing eggs were placed into small trays with hydrated chicken feed, to feed the newborn larvae. This substrate was used due to its availability in the market, its high protein content and its high palatability, ensuring them a balanced and quick development. Tray covers had a small ventilation area, in order to maintain inside the trays, the relative humidity needed to obtain a high percentage in hatched eggs. After approximately seven days, newborn larvae were transferred in open boxes and they were fed with hydrated chicken feed until the 50% of larvae became prepupae. Upon reaching this stage, they stop feeding and then they become pupae. The tanks were then covered with aerated lids, to easily collect emerging adults and to transfer them into the mating cage.

Larvae were reared on different substrates: hydrated chicken feed (control sample), tomato peels, pomace and dregs from the wine chain. Ad hoc tests were set up to obtain information about *Hermetia illucens* larval growth and mortality on each substrate in order to evaluate their suitability for mass larval production. To extract lipid and protein components and to study their antioxidant, antimicrobial activities, *Hermetia illucens* larvae were collected just before reaching the prepupae stage. The larval weight and mortality at 7, 10 and 14 days from the start were measured and every thesis was replicated four times. Larval growth on unaltered and shredded residual biomasses were evaluated in laboratory scale, omitting in this study industrial scaling-up. It worth to mention that industrial larvae rearing require space in order to allow optimal substrate conversion. The results are reported in Fig. 2.

Initially, larvae had homogeneous weight. After 7, 10 and 14 days the control larvae weight was higher than that of the residual biomasses, both shredded and unaltered ones, even if the differences mitigate after 10 and 14 days. The larvae fed with residual shredded biomasses showed a higher growth compared to the ones fed with unaltered residual biomasses, both at 7 and 10 days, but, after 14 days, there were no differences in larval weight between the two substrates. Considering the percentages, the differences in the growth are more immediate to be evaluated (Fig. 3).

The average mortality measured during the 14 days of the experiment was 0% in control and in shredded residual biomasses samples, instead it was 3.26% in the unaltered residual biomasses. In conclusion, the performance after 7 days is higher if residual biomasses are shredded. Otherwise, if the larvae are reared for 14 days, there is no significant difference between the two types of residual biomasses.

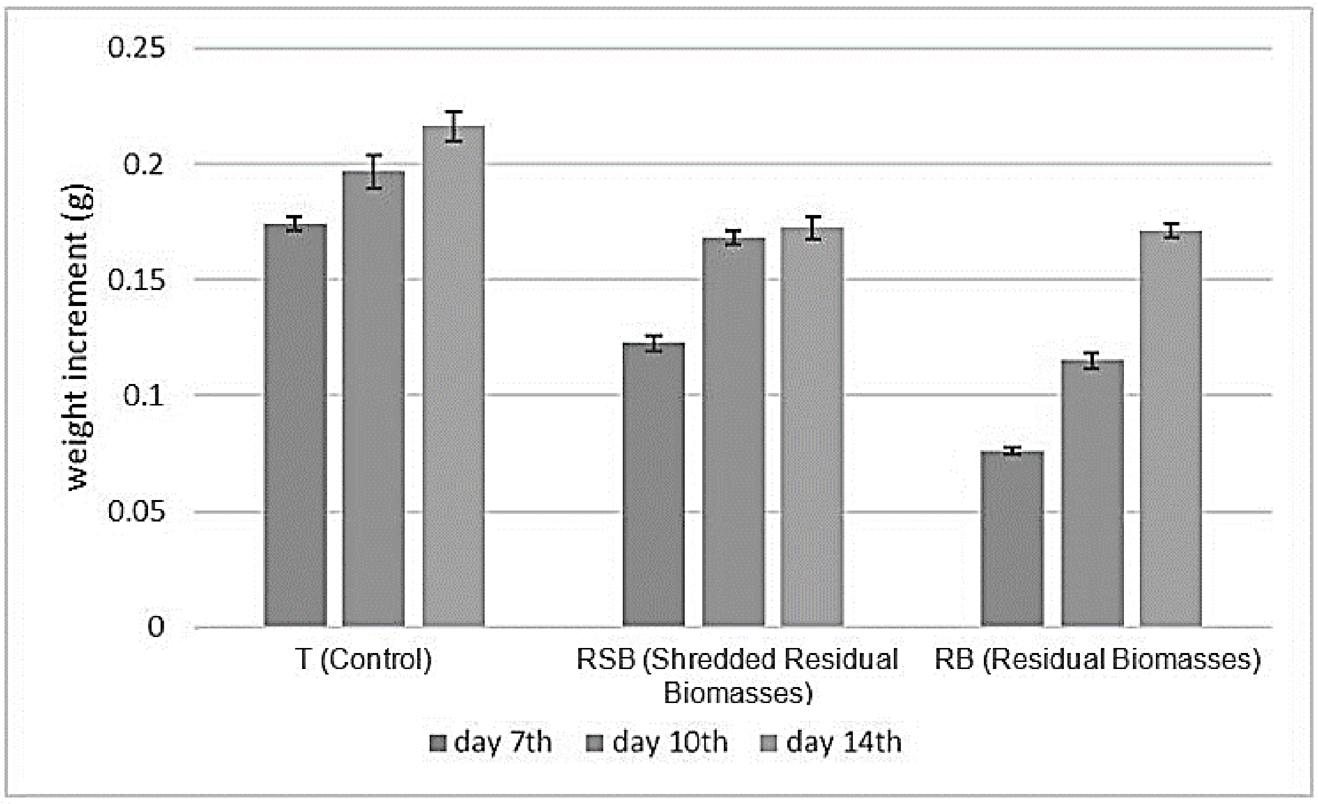

Fig. 2. Larval weight increase in control test, residual shredded biomasses test and unaltered residual biomasses test

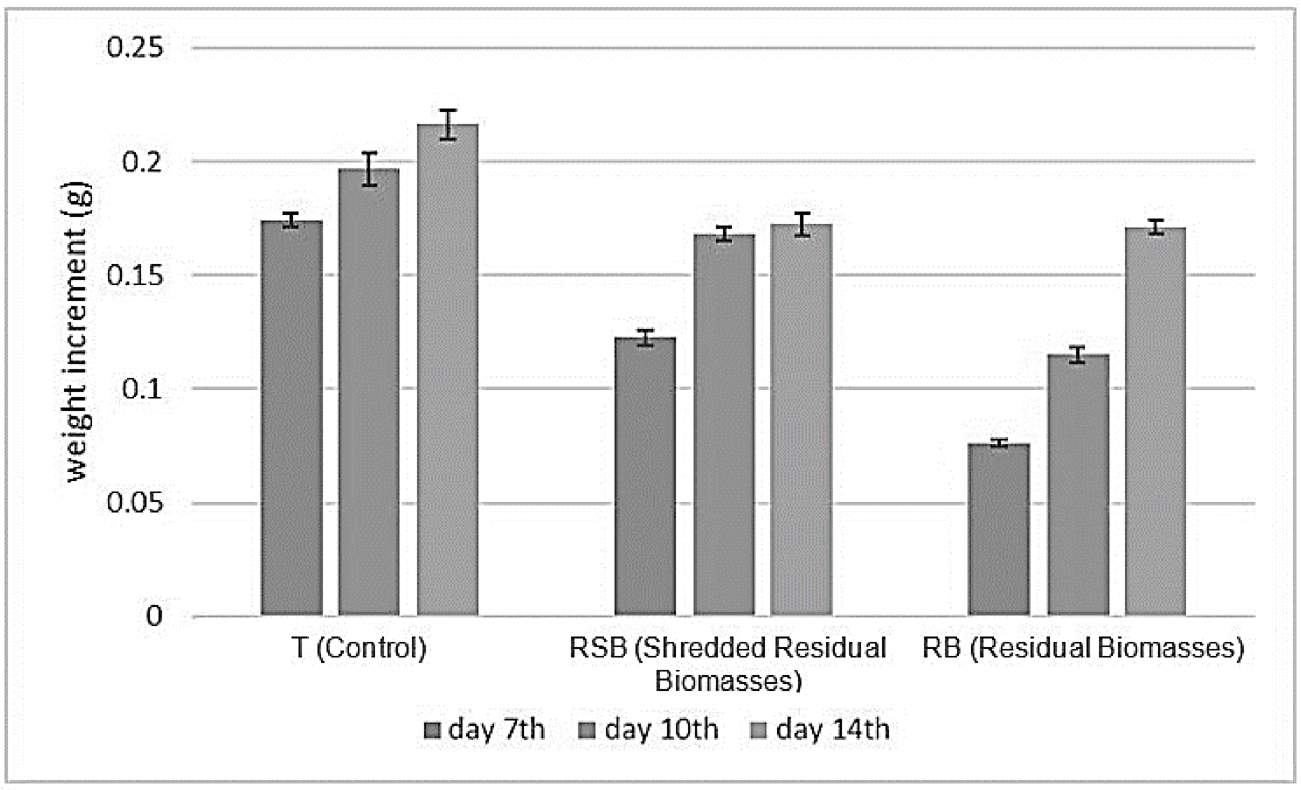

Fig. 3. Larval weight increase in control test, residual shredded biomasses test and unaltered residual biomasses test [%]

3.5. Development of eco-friendly extraction techniques for the chemical extraction of molecules of cosmetic interest

Insects provide a valid alternative to some of cosmetic ingredients, due to their high value biomass, whit high value protein and fat content (Tzompa-Sosa et al., 2014). Amongst these insects *Hermetia illucens* larvae represent a valid option as resource for cosmetic ingredients, since their fat profile is similar to natural oils that are already used in cosmetics (Verheyen et al., 2018), and since the protein and enzyme content show a high antioxidant activity (Firmansyah and Yusuf Abduh, 2019). Literature studies state that insect biomass composition varies according to species, life stage and its diet (Finke and Oonincx, 2014). In the case of *Hermetia illucens*, during larval stage, lipid content increases up to 40% and is strictly dependent on the lipid and carbohydrates content in the feeding substrate (Devic and Fahmi, 2014; Spranghers et al., 2017).

Extraction of molecules of interests from the selected residual biomasses respecting the concept of "green chemistry" is of vital importance in order to obtain a sustainable biorefinery. In order to achieve this goal, solvent extraction was performed taking into account the origins (fossil or renewable resource), boiling point and yield of extraction of the solvents. Among the solvents, MTF was selected because comes from renewable feedstock and has low toxicity on humans and environment; moreover, is considered a good solvent for fat and carotenoids extractions (Sicaire et al., 2014).

Moreover, in order to increase the yield of extraction, ultra sound assisted solvent extraction was considered among other recent technologies known to be enhancers in extraction processes.

Solvent selection for lycopene extraction led to choose for MTF in terms of yields of lycopene extracted, while solvent selection and concentration for polyphenol extraction from dregs show a high yield using 75% acetone or 50% ethanol (data not shown). Fat content of tomato peels, grape dregs and cheese "morge" resulted in 3.5%, 1.6% and 43.0% of dry matter, respectively. Protein content of tomato peels, grape dregs and cheese "morge" resulted in 15.2%, 18.1% and 47.0% of dry matter, respectively. Results show that cheese "morge" has the highest potential to be reach in lipids and proteins, while tomato peels and grape dregs a high protein content. Despite the obvious recovery of high valued molecules like carotenoids and anthocyanins, all the residues of the supply chains studied are a resource in terms of protein and peptides to be used in cosmetics formulation.

The analysis of larvae fed on tomato peels, showed a lipid content in the Soxhlet extraction with petroleum ether of 24% of dry matter (against a 21% of dry matter for group control larvae fed on chicken feed) and in the extraction with MTF of 40% of dry matter (against a 23% of dry matter for group control larvae), showing a highest yield of extraction with MTF in comparison to petroleum ether. The ultrasonic assisted extraction showed a high yield of extraction (98%), indicating the validity of the extraction method compared with the Soxhlet extraction. Soxhlet extraction has the advantage to repeat extraction process in cycles, using a limited amount of solvent that is recycled in each cycle through evaporation and recondensation.

Unfortunately, Soxhlet extraction require to operate for several hours and relatively high energy consumption to heat the solvent to his boiling point and, moreover, require a large amount of tap water for the recondensation process or energy consumption in case of high boiling point solvents. Ultrasonic assisted extraction, instead, is a valid alternative in terms of modern extraction technique, making the extraction process greener and more suitable in a circular economy approach. The characterization of lipid content from larvae revealed a content of fatty acids in the range C10 - C20 with lauric acid representing the major component among them, followed by palmitic, oleic, myristic and linoleic acids. Lauric acid has been demonstrate to have potent antibacterial and antiviral activities (Anzaku et al., 2017) and could also been easily converted into monolaurin, showing potent preservative proprieties (Ushakova et al., 2016). Verheyen and co-workers (Verheyen et al., 2018) compare *Hermetia illucens* larvae oils to other natural oils suggesting its substitution in skin cosmetic formulations. In this process is recommended to remove phospholipids and unsuitable free fatty acids, as well as to improve its color and odor characteristics.

Preliminary results on the characterization of fractionated protein hydrolysates show a higher content of the < 1kDa fraction and a lower content of the > 10kDa fraction in the enzyme hydrolysate in comparison with the other extract.

3.6. Energy and agronomic recovery of residues

The real closure of a circular economy approach can be obtained only when all the material is recycled or upcycled, for a new utilization, or used in energy production at the very end. Combustion is not an option in this case, because it destroys materials and liberates emissions, while producing some forms of energy.

In the present case study, pyrolysis, or pyrogasification, is the method for the final disposal of all the residues of the previous phases. In fact, every kind of organic material can be a feedstock for pyrolysis, as such without treatments, or else in mixtures with wood and dry biomass. The pyrolysis process is a controlled combustion at fixed temperatures (300-750°C) and low oxygen concentration, and therefore it does not incinerate the feedstock. This process always generates energy in the form of steam and heat, a syngas containing CO, CO_2, CH_4 and H_2, and a bio-oil which can be used as fuels. Most of the carbon contained in the feedstock however is preserved after pyrolysis in the form of “biochar”, in which carbon is stabilized in organic form (Joseph and Lehmann, 2009).

Biochar has a “nanostructure” with extended surfaces and cavities, deriving from the structure of the feedstock which is mostly preserved (Marmiroli et al., 2018). This extended surface is reactive due to chemical functionalization and reactive groups, and this makes the biochar an interesting material with useful properties. According to EU legislation, biochar from plant origin can be applied as a soil amendment or improver, also in organic agriculture. Biochar improves soil properties such as water retention and texture, increases the pH of acidic soils, modifies the mobility of nutrients, contributes to sequestration of organic and inorganic contaminants, and stimulates the growth of microorganisms. As a final result, it improves the growth of plants. Pyrolysis is therefore considered as a desirable process in closing the cycle in agricultural context, because the carbon contained in the residual biomass is returned to the soil as amendment, in a stable form which is not subjected to further degradation and without emissions of CO_2.

A series of guidelines are available to evaluate the biochar production and its quality (EBC, 2020; IBI, 2015). The European Biochar Certificate in particular, has been developed to become the voluntary European industrial standard ensuring a sustainable biochar production and low hazard use in agronomic systems.

Biochar will therefore represent the final product of the residual biomass of tomato, dairy and wine supply chains under study in the BIOWAFER project.

4. Conclusions

BIOWAFER will make the availability of waste and by-products of the agri-food sector in Emilia Romagna known, identifying their potential for exploitation. The project therefore exists in the context of a circular economy, producing new products with high added value (like lycopene, polyphenols, anthocyanins, lipids and proteins/peptides) and proposing alternative solutions to the traditional disposal of the residual biomasses of agri-food chains.

Thanks to a biorefinery approach that envisages consecutive and integrated processes, the valorization of these residual biomasses, provides an alternative path of qualification leading to high added value products, of potential interest for the cosmetic and pharmaceutical industries.

The use of eco-friendly extraction processes allows to reach the goal of eco-friendly biorefinery with: a) a total reduction of residues in a circular way; b) obtaining molecules of interest required by the market because they are natural and of plant origin; c) reduction of synthetic molecules; d) use of an eco-friendly solvent like MTF with higher yields of extraction. Many other circular approaches are presented in literature, but, in our knowledge, no one use fermentation coupled with larvae nursery for waste reduction and conversion.

However, one of the most challenge aspects in scaling larvae rearing on residual wastes is the space requirement: larvae in fact tend to rear on the surface of the substrate because of the lack of oxygen in the lower layers. Another important aspect to be evaluated is the potential impact factor of the rearing process of larvae on the environment. Moreover, it is crucial to address the possibility that larvae reared on fermentation residue could lead to a lower mass content (in term of lipid content) biomass due to the possible lack of carbohydrates from the rearing substrate.

The biochar obtained from pyro-gasification of the residues of all the project phases (fermentation residue, larvae nutrition substrate with larvae manure, larvae residue after defatting and hydrolysis process), which can be used for agronomic purposes, will instead contribute to increasing soil quality, by increasing agricultural yield, reducing the use of synthetic fertilizers, thus improving soil structure and its water retention capacity, with obvious positive effects also in terms of water saving. Biochar sequesters carbon in a stable form, helping stakeholders and farmers to develop more sustainable production models, which can offset other greenhouse gas-producing activities.

In future steps we will study other molecules of potential interest obtainable from the same matrices and integration with other supply chains will be evaluated. Furthermore, the economic and environmental sustainability of what is proposed will be studied as these approaches can become widely used only if truly sustainable.

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THE POREM BIO-ACTIVATOR AS A SOLUTION FOR DEGRADED SOILS: RESULTS OF FIRST ITALIAN TRIAL

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Abstract

Recent studies have highlighted those European soils are subject to high rates of degradation. Therefore, new strategies to contrast the soil depletion are required. The European project related to POREM (POREM_LIFE17-ENV/IT/333) aims to be a valid solution to the problem with the production of an innovative bio-activator, named just POREM, cheap and based on two main natural raw materials, widely available: poultry manure and a natural enzymatic preparation, derived from plants. Indeed, POREM recycles the main waste of the poultry productions and hence represents a new idea of green fertiliser, which can provide nutrients and organic matter to the soil for their rehabilitation, placing itself in a circular economy strategy.

In this work, the outcomes of physico-chemical characterisations and field application tests, related to the first-year Italian campaign of POREM production at pilot scale, were presented. The characterisation results show the bio-activator maturation over the time and the struvite presence which is a nitrogen compound, useful for N retention and for reducing environmental impact. POREM activity under field conditions on several soils was studied by field tests in Northern and Southern Italy both on vegetable and arable crops. The outcomes demonstrated a significant fertility improvement. Indeed, there are a decreasing of the needed mineral fertiliser and an increase in the yield and crops quality. The field tests planned for the upcoming year campaign will focus on the soil restoration to reduce degradation.

Key words: bioremediation, bio-activator, industrial symbiosis, poultry manure, soil restoration

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1. Introduction

Over the past decades, global climate change and human activity have led to global soil degradation (DeLong et al., 2015; Oldeman, 1991). Considering that about 45 % of the European land was at potential risk of degradation (Cerdan et al., 2010; Hill et al., 1995; Montanarella, 2007), it is crucial to found new solution to protect the soil, preserve its function and restore degraded soil (EUR-Lex, 2006). Soil degradation is understood as a set of mutually dependent factors leading to land degradation: biological, chemical, physical degradation and erosion (Johnson et al., 1997). The main consequence of this is the decline in soil fertility (Hartemink, 2006; Soil Science Society of America, 1997) that is defined as ''the quality of a soil that enables it to provide nutrients in adequate amounts and in proper balance for the growth of specified plants or crops''. The main causes of soil erosion are wind, ice, water and movement related to gravity.

Water erosion can be natural or accelerated by human activity phenomena depleting the soil structure by the action of water. The rate of erosion is not equal

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in all the lands and it is affected by several parameters depending on the soil, local landscape, and weather conditions. In particular, wind erosion is ascribable to strong winds which blow over the soils with a light texture when the drought comes. In the case of ice erosion, it means the abrasion of the land by movement of a glacier onto the ground. Physical degradation includes very different processes and morphometric forms. One of them is the deformation of the inner soil structure by compaction, caused by tracking with heavy agricultural machinery. Also, it includes the formation of crusts at the soil surface by water and wind erosion (Blum, 2011). Biological degradation of soil refers to the decrease or elimination of one or more "significant" populations of microorganisms in soil, often with a resulting change in biogeochemical processing within the associated ecosystem (Sims, 1990).

Chemical degradation is due to changing the elemental concentration of soil thus altering salinification, acidity and toxicity. The main causes of solid acidification are the use of acid-forming nitrogenous fertilisers, the deforestation and the effects of acid precipitation. Soil salinization is the accumulation of free salts; accumulation can extend so much leads to degradation of the agricultural value of vegetation and soils. It is carried out by a combination of both natural and human-caused processes. Another important phenomenon of chemical degradation involves the decrease of carbon concentration which is highly relevant to cultivated fields.

A key soil component is organic matter (SOM), which affects plant growth both indirectly and directly (Bongiovanni and Lobartini, 2006). The main SOM benefits are that it acts as a storehouse for nutrients, it is a source of soil fertility and contributes to soil aeration reducing soil compaction (Jones et al., 2005). Also, it determines the improvement of infiltration rates and the increase in storage capacity for water. Another important contribution is that SOM is a buffer that preserves the soil from rapid acid changes and it is an energy source responding to the needs of soil microorganisms (Van-Camp et al., 2004). As far as Europe is concerned, several areas have low levels of SOM; the European commission report estimates that the 74% of land in Southern Europe has "very-low/low" carbon concentration in soil (Van-Camp et al., 2004). The common strategy is to use compost to mitigate soil carbon loss associated with crop harvesting/agricultural production. (Zheng et al., 2020). However, the aim of the work is focused on the production of soil bio-activator - an association of organic matter for soil fertility and nutrients for plants/crops. The applied technique and the LIFE project are coherent with the research direction of composting technology: integration of mineral/nutrients with organic matter. But, in this case, mineral/nutrients are already inside the substrate (poultry manure) and the technique is addressed to reduce gaseous losses, both for C and N, and develop the autochthone microbial part. (Dall'Ara et al., 2019). Indeed, the simplified treatment can be performed also on farm and static process can reduce volatile compound emissions. Nitrogen is another important element needed for crops and life cycles of the ground. It is used in agronomy in order to stabilise the ground nitrogen concentration, fertilisers base on it. Phosphorus is considered of great importance during the first stage of plant development. The only soluble form of phosphorus that can be assimilated by plants is the orthophosphate ion, with a negative charge. Moreover, the concentration of magnesium, potassium, calcium and sodium determines the Cation-exchange capacity (CEC) and it affects soil fertility. The so called "microelements of soil" (Fe, Mg, Mb, Zn, Cu and B) have an essential role in the plant growth, but an excessive concentration of Zn, Mb and Cu is considered a potential pollutant and toxic for the crops.

All the country patterns of the project related to POREM, Italy (Basso et al., 2003), Spain (Van-Camp et al., 2004) and Czech Republic (Žížala et al., 2019, 2017), have a direct national interest in soil degradation. The definition of *soil degradation* is different for each country: for the Spanish soils, it is related to the plant's absence caused by erosion (rain, flood); for Czech soils to the abiotic and biological immobilization and leaching, which caused structural damage, soil compaction, surface run-off; finally, for Italian soils it is ascribable to the soil's exploitation and the resulting Low Organic Carbon percentage. In particular, our research is based on two Italian locations for field testing: Forlì-Cesena Province (Emilia Romagna region, Northern Italy) and Loc. Tertiveri, Biccari, Foggia Province (Puglia region, Southern Italy). These soils are degraded as shown by their poor carbon concentration. Indeed, the average carbon percentages reported in the data of ARPA Emilia-Romagna maps at (44.166095, 12.267886) are in the range of 1.1 - 1.3 % (Staffilani et al., 2015). Soil samples of each location were collected and analytic experimental measurements of carbon (total and organic) were carried out by Elemental Analyser LECO C, N, S technique in CEBAS CSIC Certified laboratory. The tests showed respectively a value of 1.62 ± 0.06 % of total carbon soil for the Cesena field and in the Biccari location an amount 1.4 ± 0.2 % of percentage of carbon soil. These quantities do not guarantee an appropriate grade of fertility for the crops as described in the report of ARPA Veneto (Giandon and Bortolami, 2007; Van-Camp et al., 2004). In the present work, the physico-chemical characteristic of POREM bio-activator will be analysed during its maturation. Moreover, the effect of POREM as sustainable fertiliser for degraded land will be evaluated by field tests.

2. Material and methods

2.1. POREM bio-activator production at pilot scale

According to EP1314710 (Memmi and Ridolfi, 2002), the POREM bio-activator production is carried out forming three piles of poultry manure (3ton) whose was added the Vegetable Active Principles, that is an enzymatic preparation based of plants. The piles were made under a roof, but not isolated in a room, to ensure the natural air recycling. It is an innovative, simplified and static process which allows the POREM maturation, along 120 days, with oxygen available from natural convection. For these characteristics, the process can be considered an "energy saving biotreatment" and then it is a low-cost technology. Moreover, POREM bio-activator derives from waste product of the poultry industry, widely available, which is reused, in accordance with a circular economy strategy. All these aspects influence the bio-activator cost, which is lower than other technologies (e.g. compost needs the oxygen supply and the overturning of the pile, procedure which increases the cost of technology).

The POREM bio-activator were produced in two different Italian production sites, Puglia and Calabria (hereinafter referred to as ITP and ITC respectively), to test the replicability of the bio-activator production process. ITP samples derive from poultry raised in litter and whose diet only includes seeds, while ITC samples derive from poultry whose diet provides additional calcium to help them in the eggshell formation.

2.2 POREM bio-activator sampling procedure

The POREM properties were evaluated at different maturation time: thirty (t30), sixty (t60), one hundred and twenty (t120) days and also the as prepared POREM (t0) was analysed as reference starting point. Moreover, each sample consisted of the mixing of sub-samples collected by different pile positions. Specifically, three samples were collected for each pile (e.g. samples 1.1, 1.2 and 1.3 from pile 1) and each represented a portion of the pile (i.e. 1.1➔A, 1.2➔B, 1.3➔C; see Fig. 1). Each individual sample consisted of six subsamples, collected at three different points of the same part (top, bottom and middle) and two different depths (20cm and 50cm). This sampling procedure was followed for each selected maturation time and each pile. Therefore, for each sampling time, nine samples were obtained (Fig. 2, ITP production case). Subsequently, the samples were dried and grinded by CEBAS-CSIC in order to obtain homogeneous samples. The analyses were carried out on individual sample and the final properties were calculated as the mean of the measured values.

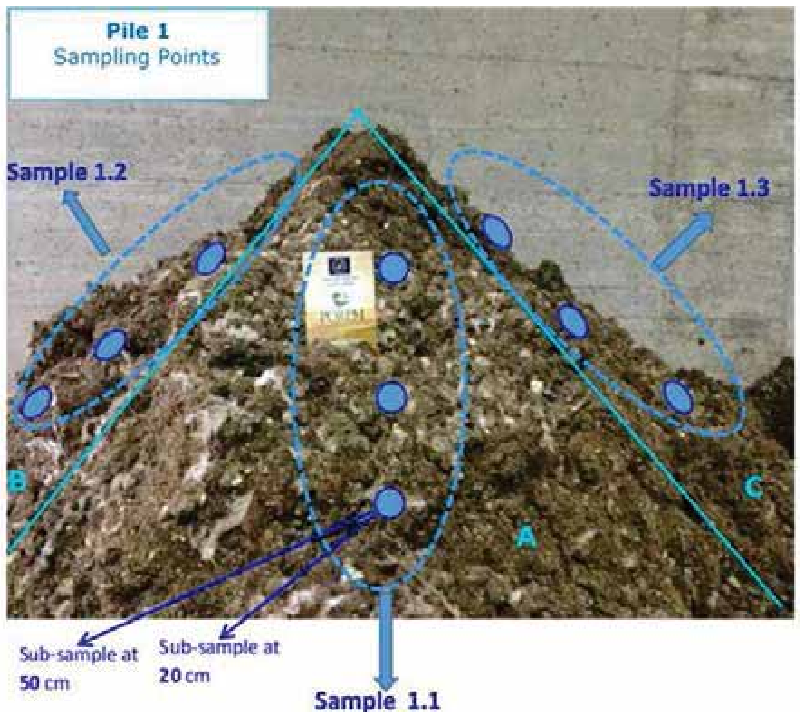


Fig. 1. Diagram of POREM bio-activator sampling (pile 1)

2.3 Physico-chemical characterisation methods

Using the Simultaneous Thermal Analyser (STA 409C, Netzsch), in Thermogravimetric Analysis (TGA) mode, the mass loss and the differential of mass loss were measured to detect decomposition phases and evaluate the thermal stability of the samples. The TGA were carried out under the following conditions: inert dynamic atmosphere (argon, 100 mL/min), heating rate of 10 ° C / min, final temperature of 1000 °C and initial mass of the sample of 850 mg.

Scanning Electron Microscopy (SEM, LEO 438 VP) was used to observe the morphology of the POREM bio-activator. Moreover, a compositional semi-quantitative analysis was carried out by Energy Dispersive X-Ray spectroscopy (EDS, ISIS 300), through the specific detector the SEM is supplied with. The average composition was acquired and, in localised areas of particular morphology, the specific composition was also obtained. All samples were characterised as received, without any pre-treatments and, therefore, avoiding any possible contamination or damage. Different areas were analysed by SEM-EDS in each sample to have more reliable and representative results.

The X-Ray Diffraction analysis (XRD, Philips PW1710, Bragg–Brentano geometry) was performed for the identification of the crystalline phases in POREM samples (CuKα 40 kV-30 mA, scan step time 3 s, step size of 0.02°).

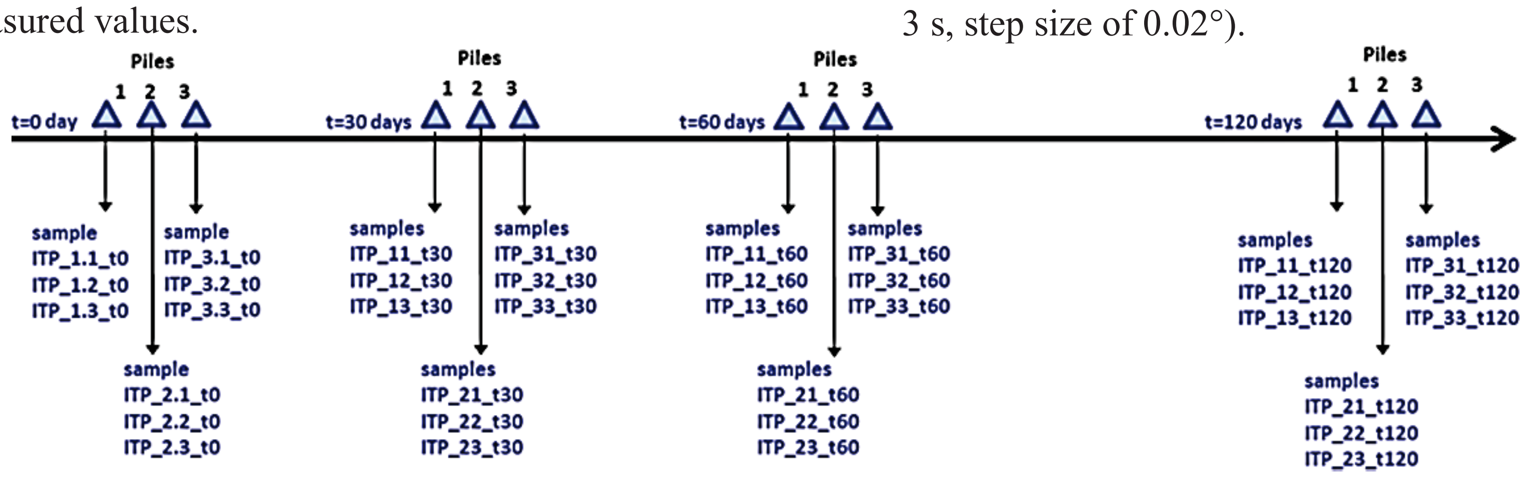


Fig. 2. Flow chart of ITP experiment

2.4 Parameters of field tests and related agricultural index

POREM bio-activator was tested on two Italian soils (Forlì-Cesena, Emilia-Romagna region and Foggia, Puglia region), described in Table 1. The aim of the experimental field tests was the evaluation of yield quantity and quality improvement obtained from crops grown in soils treated with POREM bio-activator or with standard fertilisers in comparison to crops grown in untreated soil.

Pilot field tests in Italy demonstrated improvements in terms of quantitative and qualitative production (yield) of arable and vegetable crops grown on soils treated with POREM. In Forlì-Cesena area (Northern Italy), POREM was tested on industrial tomato production under conventional farming. Crop evaluations were executed comparing the performance of POREM bio-activator (40 nitrogen units per hectare) to that of a conventional mineral fertiliser NPK 26-46-50 (130 nitrogen units per hectare), used as chemical standard reference; in addition, an area not treated (untreated check) was included in order to carry out result comparisons. The standard fertiliser amount was set in order to provide a nitrogen amount calculated on the basis of indications reported by the Emilia-Romagna Region IPM (RER Directive, 2020). This first pilot test on vegetable crops was carried out with four replicates per each treatment. The crop was evaluated by the improvement in marketable fruit production in comparison with the untreated reference and by the quality parameter of Brix degree**,** which assesses the sugar content in marketable fruits. Crop health and vigour Index, which measures the increase in plant growth or foliage volume through time after planting, was also considered. The test was replicated on barley crop and was carried out in the hills near Foggia area (Southern Italy), characterised by poor and degraded soil in organic farming.

Field evaluations and crop production were observed on the two fertilisers (POREM application at 80 kg N/ha and Bioazoto N12 at 80 kg N/ha, used as organic standard reference); an adjacent untreated area was used for comparisons in field data recording.

Table 1. Initial characteristics of Italian soils

Parameters		***FORLÌ-CESENA soil***	***FOGGIA soil***
		mean values	
pH	**-**	6.98	8.35
Electrical Conductivity	**µS/cm**	94.00	121.83
Bulk density	**g/cm³**	1.16	1.15
Aggreggates	**%**	69.17	44.51
B-Glucosidase	**µmoles PNF/g*h**	0.43	1.19
Phosphatase	**µmoles PNF/g*h**	1.48	3.45
MACROELEMENTS			
Calcium	**g/100g**	1.19	13.43
Assimilable calcium	**meq/100g**	24.89	24.34
Potassium	**g/100g**	0.76	0.86
Assimilable potassium	**meq/100g**	0.55	1.19
Magnesium	**g/100g**	0.95	0.49
Assimilable magnesium	**meq/100g**	2.82	1.12
Sodium	**g/100g**	0.04	0.05
Assimilable sodium	**meq/100g**	0.26	0.22
Phosphorus	**g/100g**	0.05	0.06
Assimilable phosphorus	**meq/100g**	21.67	8.97
Sulfur	**g/100g**	0.03	0.09
MICROELEMENTS			
Boron	**mg/kg**	36.03	24.70
Iron	**g/100g**	3.43	2.44
Manganese	**g/100g**	1076.30	1212.82
Cadmium	**mg/kg**	0.73	0.51
Lead	**mg/kg**	56.07	32.11
Cooper	**mg/kg**	40.57	29.55
Chrome	**mg/kg**	106.70	43.45
Nickel	**mg/kg**	67.17	26.25
Zinc	**mg/kg**	85.83	51.79
Total nitrogen	**%**	0.15	0.13
Total nitrogen water soluble	**ppm**	20.13	0.53
Total organic carbon	**%**	1.08	1.37
Water soluble carbon	**ppm**	167.67	237.48

In this case, each treatment was evaluated in two different field parts (upper and lower, for a total of six replicates), characterised by two different soil structure based on gravel and stone quantity. The crop was evaluated by plants improvement in number and vigour, at crop-emergence and pre-flowering, and production improvement in grain weight at harvest, in comparison to the crop grown in the untreated land. All field results were evaluated with ANOVA analysis which was performed with the ARM Software.

3. Results and discussion

The analysis of the bio-activator POREM has foreseen two phases: the characterisation to establish its intrinsic physico-chemical properties, both of Calabria and Puglia samples, and the field tests to evaluate its activity on the crop. The measures also include the error due to adverse climatic conditions, as in the case of ITC POREM samples around 120 days.

3.1. Physico-chemical characterisation of POREM bio-activator

The TGA results clearly suggested four main steps of mass loss which characterise the ITC and ITP samples (Cimò et al., 2014; Lee et al., 2017). Indeed, in the temperature range 25-220°C, water removal occurred. At around 220°C, the pyrolysis of organic matter began and ended at 550°C. This degradation occurred in two steps: the first, between 220°C and 380°C, corresponds the to the thermal decomposition of aliphatic fraction, that is the alkyl labile and carbohydrates systems; the second (380-550°C), to the decomposition and thermal transformation of aromatic moieties.

Finally, between 550-1000°C, the inorganic components of poultry manure have degraded with the thermal transformation of biogenic salts (i.e. calcium carbonate) and mineral. Table 2 summarises the TGA main results of Italian samples, over the time; each result is the mean of the samples collected from the three different piles. The comparison of the results highlighted a reduction of the organic matter over the time, particularly in the 220-380°C range, which is related to the aliphatic compounds of organic part (e.g. straw decomposition). Consistent with expectations, this trend is probably due to the bio-activator maturation: during this process, the organic fraction decreases, up to stabilise itself to the value which characterises the material.

Moreover, the fourth ITP step percentage of mass loss (i.e. the inorganic part) has grown slowly than ITC samples. This is related to the raw poultry manure composition: ITC showed a higher inorganic fraction than ITP samples due to the relevant calcite presence in the initial poultry manure, related to the hens' diet rich in Ca for the eggshell formation. The initial absence of Ca in ITP samples justifies the lower percentage of mass loss in this temperature range and the slow growth over the time, which is probably due only to mineralization. It can be assumed that the presence of $CaCO_3$ (or Ca) in ITC samples acted as an adjuvant for mineralization which, however, also occurred in ITP samples resulting in a slow growth of mass loss over the time. This effect is important because the mineralization and the related compounds can be considered a basin of soil nutrients.

As shown in Table 2, from the comparison among the samples collected from the different piles, the standard deviation is less than 1% for all the mass losses steps of ITC samples and less than 0.5% for about all the mass losses steps of ITP samples. Finally, the Table 2 shows how, at around 60 days, the mass tended to stabilise.

The main differences between ITC and ITP thermograms are well summarised and shown in Fig. 3(a) which depicts the mass loss and DTG (first Derivate of TG) of these POREM samples at t0: between 550-1000°C, the higher percentage of inorganic compound (i.e. calcite) in ITC sample compared to ITP sample; in the range 200-380°C, the double peak in ITP sample DTG, due to the litter straw, which was absent in ITC. Indeed, this region is typical of hemicellulose and cellulosic components. Finally, to demonstrate the homogeneity of POREM production, the replicability was also studied at piles and samples level.

Table 2. Comparison among the Italian POREM mass losses [wt%], over time

Sample Name	Mass Losses [wt%]		
	[220-380] °C region	[380-550]°C region	[550-1000]°C region
ITC t0	36.6±0.6	13.7±0.8	9.5±0.4
ITC t30	28.8±0.7	11.6±0.4	13.7±0.9
ITC t60	27.3±0.4	12.5±0.8	13.1±0.8
ITC t120	19.9±0.2	8.7±0.3	16.9±0.5
ITP t0	37.7±0.1	10.6±0.4	6.8±0.2
ITP t30	36.0±0.5	11.2±0.1	7.6±0.3
ITP t60	35.7±0.3	11.9±0.2	7.7±0.1
ITP t120	33.0±0.4	11.0±0.1	7.5±0.2

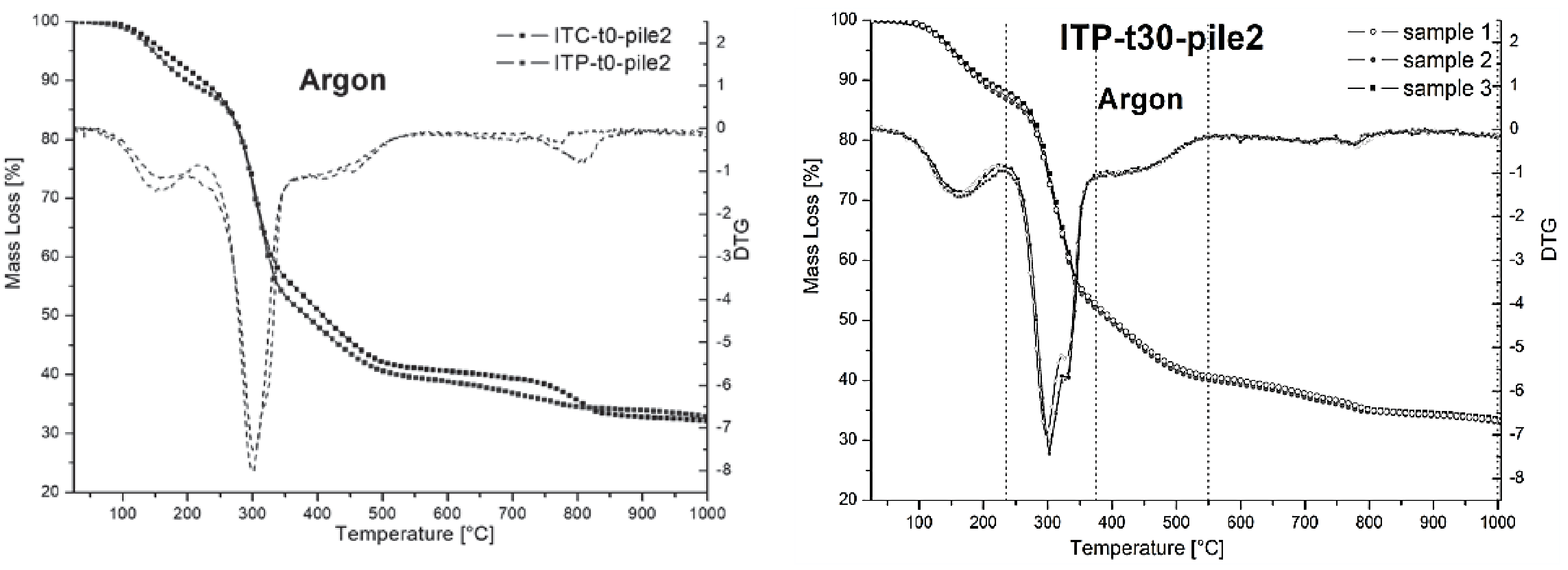
As depicted in the typical comparison between the three samples collected from the same pile shown in Fig. 3(b), the thermograms are well overlapped. Therefore, the properties showed a great level of replicability. The bio-activator morphology was heterogeneous and the micrographs showed several residues such as fibres and different shaped particles (Fig. 4a). Moreover, it was possible to identify specific particles performing localised microanalysis, as shown for calcium salt in Fig. 4b.

The production process of the POREM bio-activator was replicated at different level (sample and pile), showing similar composition with no significant variations. All samples are mainly composed of C and O, but also soil nutrients (Ca, P, K, Mg, S, etc.) are present in small quantities. The analysis of the three piles in both sites at any maturation time was averaged to show more clearly the composition trend of each element over the process.

The composition trend during the POREM maturation was shown in Table 3. The reported values were very stable over time, highlighting a remarkable process uniformity (the only data slightly out of range, Si in ITC sample at 120 days, may have been caused by the adverse conditions that occurred in Calabria around 120 days. Presumably, the rain could have dragged small percentages of sand, close to the pile, which may have been detected in the analysis). The results showed similar composition during the maturation process in both the sites, except for some differences due to the farm and hen's type.

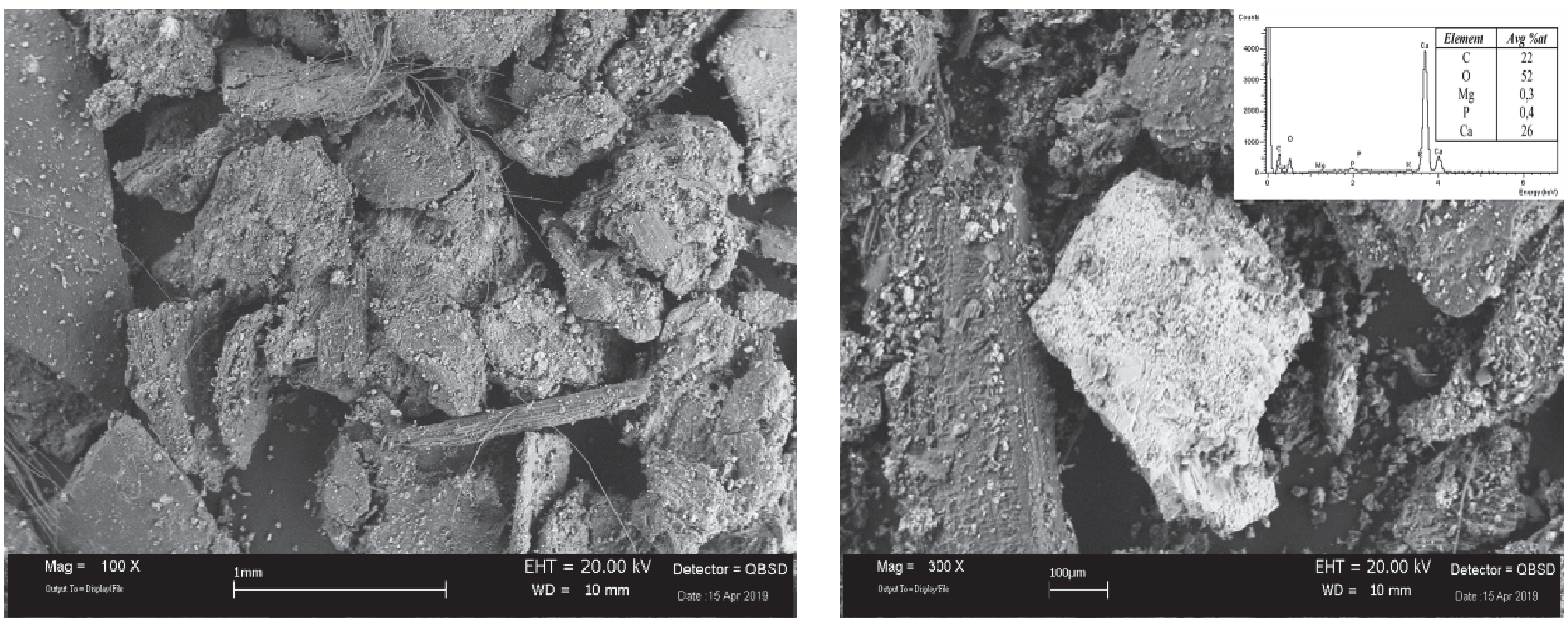
In general, the inorganic fraction increases with time. More specifically the carbon amount does not exhibit too remarkable variation. This observation, combined with the stability of calcium content, could be also an indication of calcite ($CaCO_3$) formation and C retention with consequent CO_2 evolution reduction and therefore benefits from an environmental point of view. Moreover, nitrogen is unfortunately not detectable because its EDS peak energy is between those of C and O and their high intensity completely hides that of N. However, the persistence of P and Mg contents could be an indirect sign of the struvite ($NH_4MgPO_4 \cdot 6H_2O$) formation. If so, the precipitation of N into struvite crystals would not allow a large amount of nitrogen to be released into the environment as ammonia or nitrates with a gain for the environmental impact also in this case. Finally, the presence of other elements, such as S, K, Na, Cl still at the end of POREM maturation process, is promising for its application as soil bio-activator.

The POREM bio-activator samples were composed from both amorphous and crystalline phases (Fig. 5). ITP XRD patterns shown a considerable presence of the amorphous, ascribable to the litter straw derived from the origin manure. The high content of amorphous phase hid peaks of the crystalline phases and calcite and struvite were recognised as main phases, as showed in Fig.5 (a). Instead an amorphous phase decreasing was evident for ITC samples at maturation time increasing; the crystalline main phase consisted of calcite and struvite while weddellite ($Ca(C_2O_4) \cdot 2H_2O$) was recognised as secondary phase, probably due to a manure derived by calcium rich diet (Fig. 5b).



(a) (b)

Fig. 3. Typical POREM bio-activator thermograms and relative derivate: Comparison between ITC and ITP, piles 2, at t0 (a); Comparison among the three samples of ITP piles 2, at t30 (b)



(a) (b)

Fig. 4. Typical POREM bio-activator morphology (a) and specific particle with localised microanalysis (b)

Table 3. Average elemental composition of POREM bio-activator during the maturation

	Calabria				*Puglia*			
Element	***t0***	***t30***	***t60***	***t120***	***t0***	***t30***	***t60***	***t120***
C	49±2	52±1	52±4	40±8	54±4	49.1±0.5	47.2±0.8	51±3
O	45±1	41.3±0.7	41±3	48±5	40±3	43.15±0.04	44.8±0.7	43±2
Na	0.29±0.05	0.25±0.04	0.30±0.03	0.4±0.1	0.48±0.08	0.52±0.04	0.51±0.02	0.51±0.07
Mg	0.5±0.2	0.56±0.01	0.58±0.08	0.9±0.3	0.48±0.06	0.60±0.07	0.59±0.01	0.5±0.1
Al	nd	0.02±0.02	0.08±0.05	0.3±0.3	0.2±0.1	0.22±0.08	0.11±0.06	0.11±0.04
Si	nd	nd	nd	0.2±0.2	0.5±0.1	0.8±0.2	1.0±0.1	0.6±0.1
P	1.1±0.2	1.35±0.09	1.2±0.1	1.9±0.6	1.0±0.1	1.2±0.1	1.24±0.02	1.0±0.2
S	0.29±0.02	0.30±0.02	0.29±0.03	0.4±0.06	0.35±0.01	0.38±0.01	0.43±0.04	0.45±0.06
Cl	0.14±0.04	0.17±0.05	0.21±0.01	0.25±0.03	0.5±0.1	0.60±0.07	0.54±0.05	0.54±0.06
K	1.2±0.2	1.12±0.07	1.2±0.1	1.8±0.1	1.3±0.1	1.55±0.08	1.56±0.04	1.5±0.2
Ca	3.2±0.8	3.4±0.4	3.6±0.6	5±2	1.5±0.3	1.9±0.2	1.9±0.1	1.6±0.3

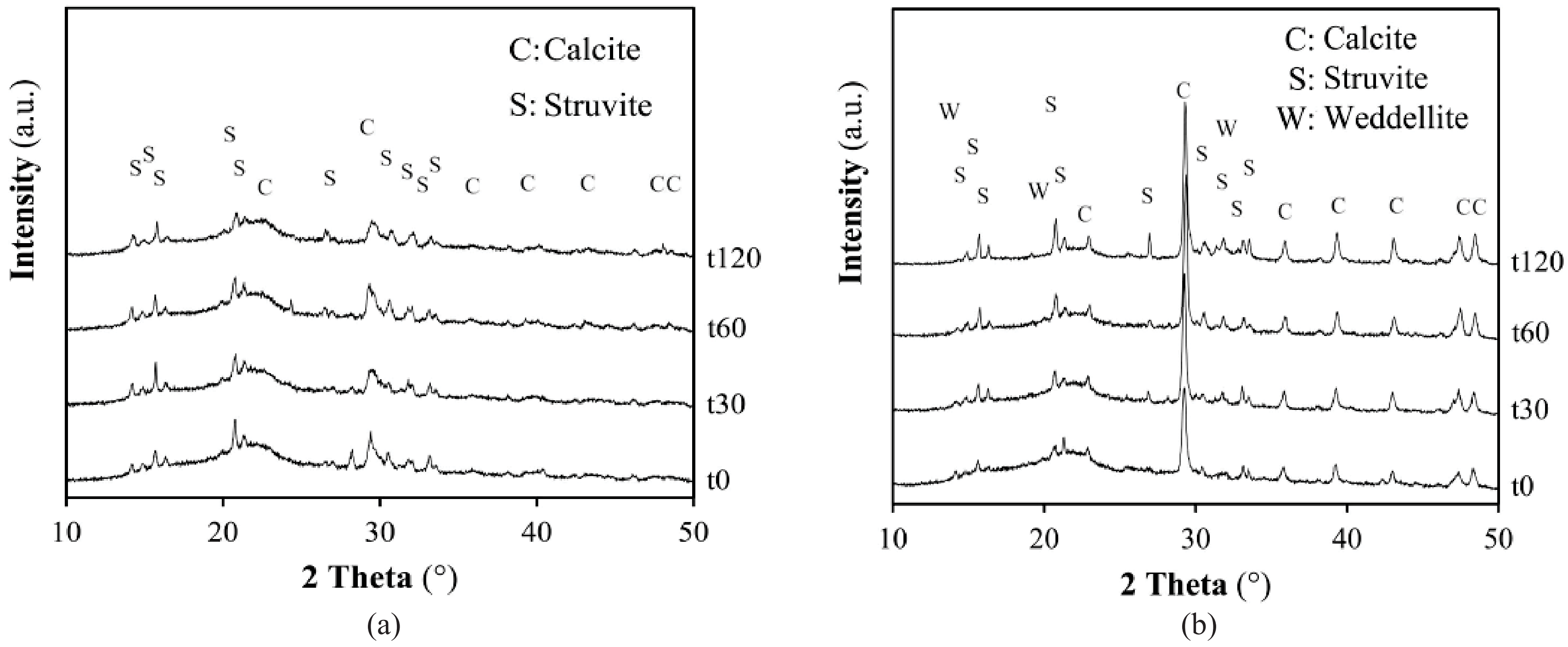


Fig. 5. Typical POREM bio-activator XRD patterns of ITP (a) and ITC (b) samples at different maturation time

3.2. Effect of POREM bio-activator application: field tests

On the vegetables pilot test in Forlì-Cesena area, the industrial tomato crop treated with POREM obtained a significant increase of marketable crop production and quality, overall crop status and biomass (Normalised Difference Vegetation Index) with respect to that of plants grown without fertiliser. The field assessments were carried out in all replicates per treatment and each parameter data are summarised in a table as overall mean (only significant parameters are presented, Table 4; please note: in ANOVA method, the same letter ("a" or "b") is used to identify values not significantly different; P=.05, Student-Newman-Keuls). Field data proved that the tomato crop treated with POREM obtained a yield statistically comparable to that treated with a mineral fertiliser commonly used in the area.

Particularly, the crop production treated with POREM reached values of sugar content of the berries (°Brix) which were significantly higher than that fertilised by a standard fertiliser, with products of mineral origin, resulting in an improvement in the commercial value of fruit production, recognised by processing companies. Overall trend of results on plant observation confirmed the POREM effectiveness in comparison to untreated, with higher leaf development and a superior ground coverage by plants, statistically comparable to that with the mineral fertiliser. In all the parameters assessed at the beginning of crop growth, POREM provided a general better performance ("starter effect") in comparison to the standard fertiliser, with a lower quantity of available applied nitrogen.

On the test on cereals (barley crop), in Southern area (Puglia) plants grown on soil treated with POREM obtained a significant increase of marketable crop production with respect to that of plants grown without fertiliser, and even superior to the conventional organic fertiliser in terms of plants emerged, overall crop status and absence of yellowing on foliage. For barley test, the assessments were carried out in both single field parts; each parameter are summarised as overall mean with six replicates per treatment (Table 5; please note: in ANOVA method, the same letter ("a" or "b") is used to identify values not significantly different; P=.05, Student-Newman-Keuls).

Field data on barley showed a similar or even superior production on soil with POREM in comparison with that obtained with a conventional organic fertiliser in a land area characterised by a high quantity of gravel and stones.

Table 4. Assessments on marketable production on tomato (vegetable crops, Emilia Romagna)

Treatment	*Fruit production [g/plant]*	*Production improvement [%]*	*Brix index [°Brix]*	*Brix index Improvement [%]*
Untreated check	1359.4 [b]	Reference [b]	4.9 [b]	Reference [b]
Standard fertiliser	1926.2 [a]	+42 [a]	5.2 [a]	+7 [a]
POREM	1813.5 [a]	+33 [a]	5.6 [b]	+16 [b]

Table 5. Assessments on ground cover and marketable production on arable crops (barley, Puglia)

Treatment	*crop-emergence [plants/sqm]*	*Plant improvement at crop-emergence [%]*	*pre-flowering [plants/sqm]*	*plant improvement at pre-flowering [%]*	*Production [g/plant]*	*Production improvement [%]*
Untreated check	236 [b]	Reference [b]	257 [b]	Reference [b]	1026.5 [b]	Reference [b]
Standard fertiliser	220 [a]	7 [a]	236 [a]	-8 [a]	1629.0 [a]	+37 [a]
POREM	281 [b]	+19 [b]	300 [b]	+17 [b]	1943.3 [a]	+47 [a]

POREM provided on barley crop an initial general better performance on the parameters observed ("starter effect") in comparison to the standard fertiliser, obtaining better results although with equal amount of available nitrogen. The comparison of results obtained in the lower and upper land parts of the field, showed that the "likely lower fertility", observed in the 'upper' land, linked to the structure of the soil including a higher quantity of gravel and stone, mostly influenced the performance of POREM. Based on these considerations, POREM showed a superior performance since the crop emergence up to harvest than standard fertiliser, providing a more evident bioremediation effect in degraded soils. Finally, the innovative bioremediation fertiliser POREM is proposed as a sustainable fertiliser to be used particularly in degraded land.

The main positive effects of the bioremediation POREM development and application can be resumed as an improvement in the ecologically friendly and sustainable crop production.

4. Conclusions

The first POREM production in Italy and its application have highlighted the intrinsic properties of the bio-activator which potentially made it useful for the plants and the soils. Indeed, it appeared as a product rich in micronutrients and carbon, natural and obtained from an innovative, sustainable and natural process which reuses the by-product of poultry industry.

The physico-chemical properties of POREM bio-activator were time-dependent until around 60 days when they showed a tendency to stabilise; this effect, related to the maturation, can be consider an indirect demonstration of the innovative, static and simplified process efficacy. As well as the stability, the replicability was demonstrated at different levels (sample and pile) and it confirmed the POREM process efficacy.

The mineralization also had an evolution over time. It is important because the mineralization can become a basin of nutrients, i.e. P or N, fundamental for the soils. Indeed, field tests have highlighted that POREM applied to soil provides a bioremediation effect, especially in "poor" and degraded land. POREM provided on both cereal and vegetable crops an initial general better crop performance ("starter effect") in comparison to the standard fertiliser, showing to be generally more efficient with an inferior or equal quantity of available nitrogen applied. The struvite presence constituted a N basin which became available.

Finally, the Italian field pilot tests showed positive results after POREM application to the soil: the crop growth and harvested product quality and quantity were better, compared to unfertilised and standard fertilised soils.

Future developments provide for replication of this experimental campaign, to confirm results and also to evaluate soil quality improvement after repeated POREM applications. Moreover, the comparison and analysis of after-applied results collected from Italy and the other European places will be also the subject of future investigation.

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EXPLORING THE POTENTIALS OF APPLYING THE CIRCULAR ECONOMY FOR WASTE MINIMIZATION AT A REGIONAL SCALE BASED ON BIG DATA ANALYSIS

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Abstract

Although significant achievements have already been made in waste recycling, the quantity of material residues that annually end up in landfills is still regarded as an important environmental pressure at the global level. This paper presents the development of a methodology for studying the potentials of resource recovery for regions and provinces with a case study in the Province of Brescia. The provincial waste management database was used for mapping the wastes' origins and destinations. A Big Data Analysis approach was followed by developing two software packages. The first package is designed in the Powerbi environment to analyse waste management in each waste category, sector, and zone. The second tool was developed using R statistical software for preparing the mass-balance models in combination with spatial analysis. The two packages provide the possibility for planning interventive actions such as the circular economy and industrial symbiosis by identifying the most problematic points and targeting the improvement measures to minimize waste disposal.

Key words: circular economy, industrial symbiosis, recovery, waste management

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1. Introduction

Circular economy (CE) is becoming one of the main sustainability strategies among various nations, and it is also considered by international organizations such as the European Union (EU) as one of the focal points in the policy documents on sustainable development (Ignatyeva et al., 2021). One of the recent and frequently cited definitions indicates that "CE as a new model of economic development promotes the maximum reuse/recycling of materials, goods, and components in order to decrease waste generation to the largest possible extent. It aims to innovate the entire chain of production, consumption, distribution, and recovery of materials and energy according to a cradle-to-cradle vision" (Ghisellini et al., 2018). CE is represented in varying ways and through different conceptual models (Kirchherr et al., 2017). The references to reuse and recycling in these models demonstrate that achieving improved performance in waste management (WM) has a deep link to the CE (Pinter et al., 2021).

On the other hand, the concept of recovery in WM as an alternative for disposal (especially landfilling) may be linked to circularity (EPA, 1999). Moreover, several indicators have been proposed for measuring CE in different contexts (Geng et al., 2012; The Ellen MacArthur Foundation, 2019). In a study by

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Sánchez-Ortiz et al. (2020), it was argued that among various indicators, those focused on WM could be more feasible to be measured in Europe. The indicators were *Waste diversion from landfills*, *Generation of waste* (*in production activities*), *Waste generation* (*in consumer activities*), and *Recycling rate for different types of waste/materials*. For the EU, these indicators are available in terms of total waste generation for economic activities (Eurostat, 2019, 2021). Ranjbari et al. (2021), in their thematic categorization of scientific publications about WM, have identified the above-mentioned indicators (i.e., waste generation, recycling rate, waste-to-energy, and recovery of secondary raw material) as subtopics under Municipal solid waste. This shows that the numerical studies for other types of wastes are still limited. Moreover, Kaza et al. (2018) has shown the current state of the recording of waste flows at the global level in different geographical contexts and the existing limits. Improvement and incentivizing of WM from recycling to the top of the waste hierarchy by the usage of IT tools is identified as an important future direction that can contribute to CE transition (Ranjbari et al., 2021). Therefore, it would be significant to develop and expand the current methods for the quantification of those fractions of generated waste that still end in landfills and to attempt to provide valorization solutions for them.

On the other hand, not only the general share of recovery for a detailed assessment of circularity is needed, but also the share of different valorisation options should be differentiated and weighed against each other. As a result of recently developed waste policies, the records related to WM in many national territories, including the EU, are collected and reported annually in aggregated forms. Due to the high amount of information in these databases, the current trend in their usage is focused on aggregations for national territories. Therefore, appropriate tools are required for disaggregating and presenting separated analyses for smaller regions or specific industrial sectors and to deal with the possible resulted uncertainties (Šomplák et al., 2019).

The flow mapping of waste streams is introduced in industrial symbiosis literature as "uncovering processes" (Chertow, 2007). However, flow mapping does not necessarily follow big data analysis since the movements of waste may be recorded by other tools such as directly visiting companies in small districts. In this case, it would be possible to characterize each waste stream by its precise physio-chemical composition, and further characterization may be asked from the owners (waste generators). However, in larger territories mapping the waste streams may be facilitated by using the local authorities' records. An application of this approach was published for industrial symbiosis study in Lisbon metropolitan area using coding systems for economic activities and waste categorization (Patrício et al., 2015). In Czech Republic, Šomplák et al. (2019) have studied some of the uncertainty problems from working with aggregated WM datasets in order to provide thematic maps for assessing each region's role in the production, recovery, and disposal of waste. Also, in Italy, coding systems were used for recording the possibilities of waste exchange among companies at regional scale (Cutaia et al., 2015a, 2015b; Luciano et al., 2016). The approach which was followed in these studies is based on engaging the interested companies for reporting their wastes (by-products) or potentially required resources in operative meetings for resource exchange. More recently, Van Capelleveen et al. (2021) considered the potential usages of waste classification tags to develop a matching procedure for industrial symbiosis by the provision of a thesaurus for the European Waste Catalogue (EWC) which may be a supplement tool for analysing WM databases. In vast areas a combination of statistical methods and spatial analysis may be useful in tracing the contribution of each sub-region unit to the whole system's performance and for programming the improvement actions (Richter et al., 2021). The following aspects can be regarded as areas for further scientific contribution:

- Provision of tools for analysing the regional datasets about WM considering the uncertainties in disaggregating procedures;
- Defining a set of parameters and indicators for analysing the potentials for developing CE initiatives;
- Assessing the limits of this approach and the data which should be exploited from other sources to have a comprehensive evaluation;

This paper presents a method for analysing the local WM systems and mapping the individual waste flows by defining a set of parameters which may be used as a framework for exploring the potentials for applying CE solutions. The provided tools and relevant metrics can support decision-makers at the regional and local scales to evaluate industrial areas' performance in the pathway toward circular economy.

2. Material and methods

2.1. Case study

The Province of Brescia covers an area of 4786 km^2 with 205 municipalities in the northern region of Lombardy (Italy). Brescia is an area historically known for its pioneer role in industrial recycling and recovery activities. Application of the symbiotic system for waste heat recovery from steel-making companies and also the treatment plant for recovery of energy from solid waste are important examples at the international level (Ramirez et al., 2017). In 2017, there were 119,972 companies in the province including large and medium industries, and also small artisanal units (Chamber of Commerce, 2017). In 2018, 9312 firms, mainly the larger and medium ones, reported their WM performances, with almost 40 % classified as manufacturers (ARPA Lombardia, 2020, 2021). The manufacturing system in the province of Brescia is mostly based on metal working and steel-making activities. Therefore, the main types of waste generated and managed in the province belong to these sectors. In Italy, the records of WM have been collected since the late 1990s in a system known as the Single Model of Environmental Declaration, in Italian as "Modello Unico di Dichiarazione ambientale", or MUD (ISPRA, 2019). The information derived from the database needs to become disaggregated to assess the performance of smaller geographic areas and evaluate the specific contribution from an industrial sector or a class of waste to the WM cycle.

2.2. Data collection procedure

In order to assess the data about WM for the study area, we first studied the data available in open-source platforms. The open-source data are generally available in the aggregated form at the regional scale. Some details may also be found about WM in provinces. For the municipalities as the smaller entities inside the province, it was impossible to find open-source data regarding their performance. This was also the case with smaller industrial districts. Moreover, the information about the performance of industrial sectors and various types of waste may only be found on aggregated scale. This means that the data about industrial activities was available for the first two digits of their ATECO 2007 codes (equivalent to European NACE codes). For waste categories, the information for larger waste families, the first two digits of CER codes (Catalogo Europeo dei Rifiuti) identical to ECW was available. Therefore, the first consideration for data collection was bringing more options for reconstructing the actual condition based on the following criteria:

- sector-based analysis
- zone-based analysis
- wastes type analysis

In each case, the limits and potentials in the usage of local databases and possibilities for improvement were assessed in collaboration with experts from local industrial associations. Following the preliminary assessment of the required information, the annual records on WM for the province of Brescia were requested from the regional environmental agency, ARPA Lombardia. In order to perform the analysis with better reliability, data for a 3-year period was collected. Each company, as a producer, transporter, recycler, or disposer of waste, is obligated to report its activities. Based on the content of the reports, the database is structured in five main sections with 30 interconnected lists of data (Ecocerved, 2020).

The main five sections include: (a) contact information of companies and their WM authorizations, (b) special wastes, (c) electrical and electronic equipments (WEEE), (d) packaging materials, (e) end-of-life vehicles. The section about special wastes contains seven lists which are coded as BA, BB, BC, BD, BE, Da, and DB. The mass flow model which is provided in this paper uses four files from this group. In order to provide a detailed example of the model structure, the contents of these files are introduced in Table 1.

2.3. Data analysis methods

Before disaggregating the collected data, a preliminary study was undertaken in light of insights from local authorities' annual environmental reports. A list of questions about the WM performance was prepared, which could not be answered with reference to aggregated data. This way, the targets of the data analysis were defined. These points were the followings:

- input-output mapping of the study area as a black box in order to show the relationship between the area and its surrounding regions
- mapping the WM network among the smaller elements such as sectors, districts, zones, etc. inside the area

Table 1. Characteristics of lists in MUD database which were used for the mass flow model (Ecocerved, 2020)

Lists	*Description*	*Types of presented data*
BA	Summary of individual companies' performance for each of their waste codes	Quantities of waste generation, delivery, transportation, or treatment carried out by the company on a specific waste code
BB	Delivery of waste between pairs of companies	Quantities of waste delivered between the two companies and their geographical location
BD	Disposal operations by treatment plants on each single waste code	Quantities of waste sent to disposal operations; D1-D15 (Eurostat, 2013)
BE	Recovery operations by treatment plants on each single waste code	Quantities of waste sent to recovery operations (R1-R13)

For this reason, it was decided to undertake these two targets by developing two software packages. The first package focuses on assessing the performance of the area as a black box with its input and outputs from the other regions. This will follow a mass-balance model with possibility of visualizing the same flows on geographical maps (Fig. 1). The second software package was developed for assessing WM in sub-systems such as municipalities and sectors to provide a user-friendly environment for supporting the first one in subsetting the bigger regional dataset (Fig. 2). For the first package, the collected information was imported to the R software for general data management and statistical analysis (Dayal, 2020). Data management was needed for preparing the data for further applications. Appropriate functions were defined, which provide the required flexibility for calculating the WM system's performance considering each study criterion.

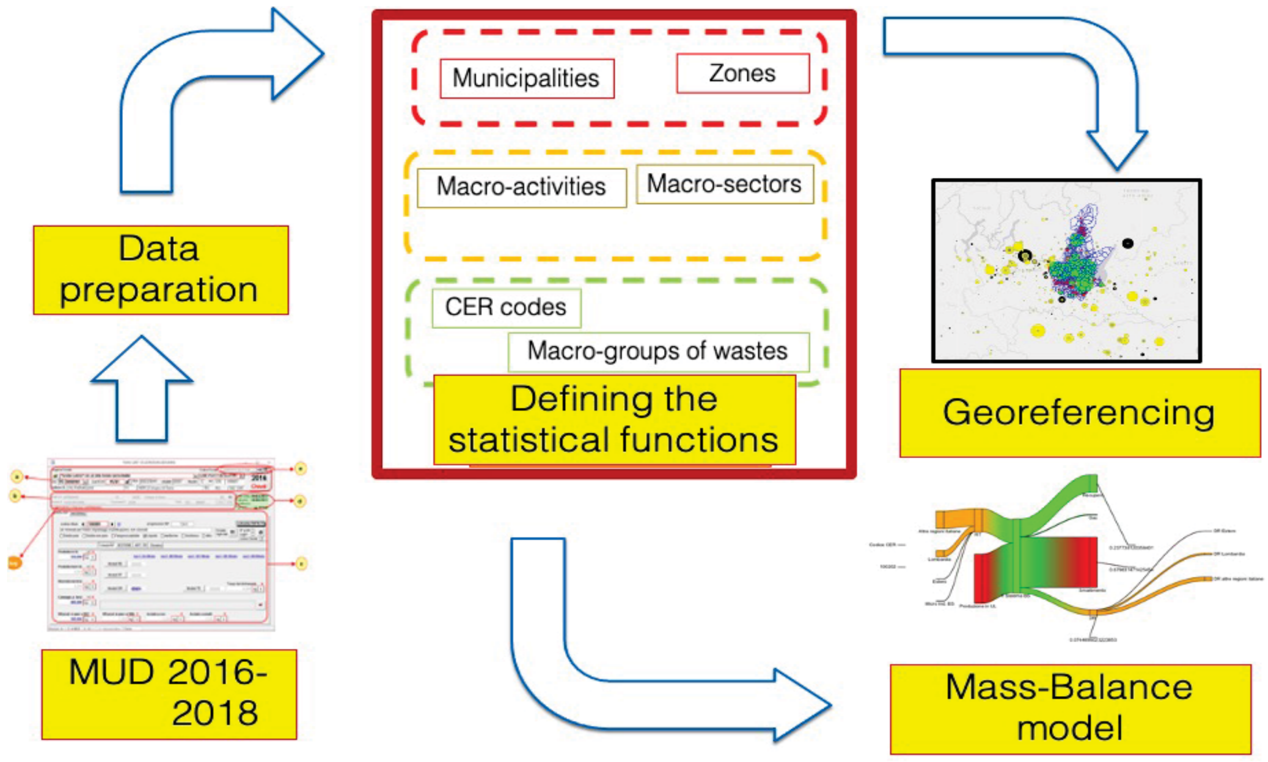


Fig. 1. The procedure for assessing the performance of the province of Brescia in waste recovery based on input-output analysis approach

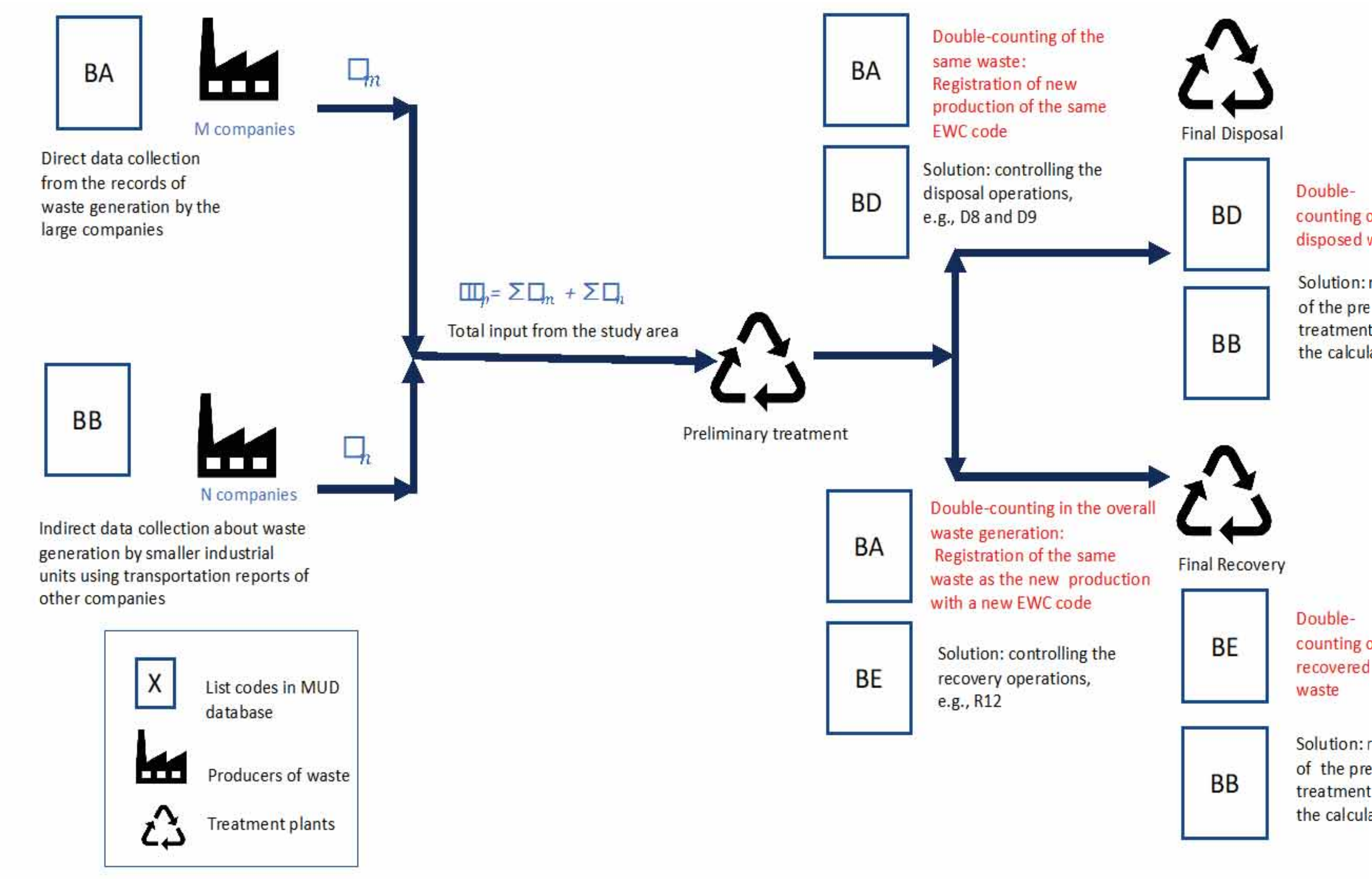


Fig. 2. Procedure for resolving uncertainty issues in the calculation of the total input of the system and assessing the destination of waste flows

The functions were defined in the form of input-out balance over the whole cycle of production, recycling and disposal. The mass flow model attempted to investigate the balance over the inputs and outputs of the WM network for each single EWC code. However, several potential sources of uncertainties existed in the database. Firstly, the treatment plant could transfer the waste after some initial treatment to a second plant. In these cases, if it underwent some changes in its physical and chemical state, the second flow may be reported as a new production by the treatment plant either with the same waste code (e.g., after a D8 operation for sludges) or with a new one (e.g., after R12 operations). Therefore, the second production report may cause a double-counting if it would be simply added to other productions. The same may occur in calculating the total treated waste if the intermediate treatments will be included in the output calculated by the model. Therefore, the model removes the double-counting cases. Moreover, there were small companies which had not to report their WM performance in the regional database according to law, while their share may be found in the BB records by waste transporters or by who received the waste for treatment. This amount of waste has also to be added as a part of the local input and differentiated from what is received from outside. An example is provided in Fig. 2, focusing on uncertainty issues and procedures for calculating input and output parameters.

The final output of the model (Fig. 4) was defined based on Sankey diagrams for evaluating the performance of the whole province as a system (Ruiz-Puente and Jato-Espino, 2020; Van Ewijk et al., 2018). The diagrams were generated by using the Sankey library of R software (CRAN, 2017). Fig. 4 shows that the total input (IN) of the system consists of two elements, waste production in the local companies and received waste from other producers (RT), which might be small artisanal units and non-industrial entities inside the province (Micro ind.). The sum of these quantities represents the system's inputs from the case study region (IN_p). The rest of the input ($IN – IN_p$) includes wastes received from companies in other provinces of the Lombardy region ($RT_{regional}$), companies in other Italian regions ($RT_{national}$), and companies outside the national territory ($RT_{internat.}$). Meanwhile, the total output (OUT) of the system consists of four main elements. Disposal (D_p), recovery (R_p), and temporal storage form the total management in the case study region (M_p). The rest of the output includes delivery of waste (DR) that may be sent to other provinces in the region (DR regional), other Italian regions ($DR_{national}$), or other countries ($DR_{internat.}$).

Comparing these parameters with the CE indicators proposed by Sánchez-Ortiz et al. (2020), four metrics were provided for assessing the CE transition in each sector or over each specific waste code:

(1) R_p/OUT = Material recovery inside the province

(2) D_p/OUT = Disposal of waste in the province

(3) $(DR_{national} + DR_{internat.})/OUT$ = Transportation of waste outside the regional boundaries

(4) IN_p/IN = Generation of specific waste in the province in total input

The presence of a potential scenario for recovery in the case study area (R_p>0) while the quantity of material recovery in the WM is minimal ($R_p << M_p$) can be investigated as an alerting sign from a non-technical barrier against CE transition which would need an in-depth study. For mapping the physical distances of waste exchanges, a spatial analysis was also supplemented using the open-source software tools in R and QGIS (Kaya et al., 2019). For this reason, all the industrial units in the database were georeferenced, and the records of exchange between them were translated to interactive geographical maps using libraries tmap and leaflet in R environment (Martorell-Marugán et al., 2021).

For the second part, the imported data from MUD dataset was prepared with Python. The cleaned data was then imported to a dashboard-base package in Powerbi. The software interface for this package is divided into eight main sections, i.e., (1) the hierarchical structure of activities, (2) the hierarchical structure of waste codes, (3) code search boxes, (4) text search boxes, (5) various graphical representations, (6) waste quantity, (7) geographical map, and (8) municipalities' slicers (Fig. 3).

The hierarchical structure of economic activities was used in this pocket for developing a user-friendly search tool for categorization of waste streams based on sectors. Therefore, this package provides an auxiliary tool for sub setting the data for geographical zones, industrial sectors, or waste codes of interest in a user-friendly environment (Fig. 6). The extracted data can then be imported as a small CSV file to the first tool for mass flow analyses and measurement of the WM circularity indicators.

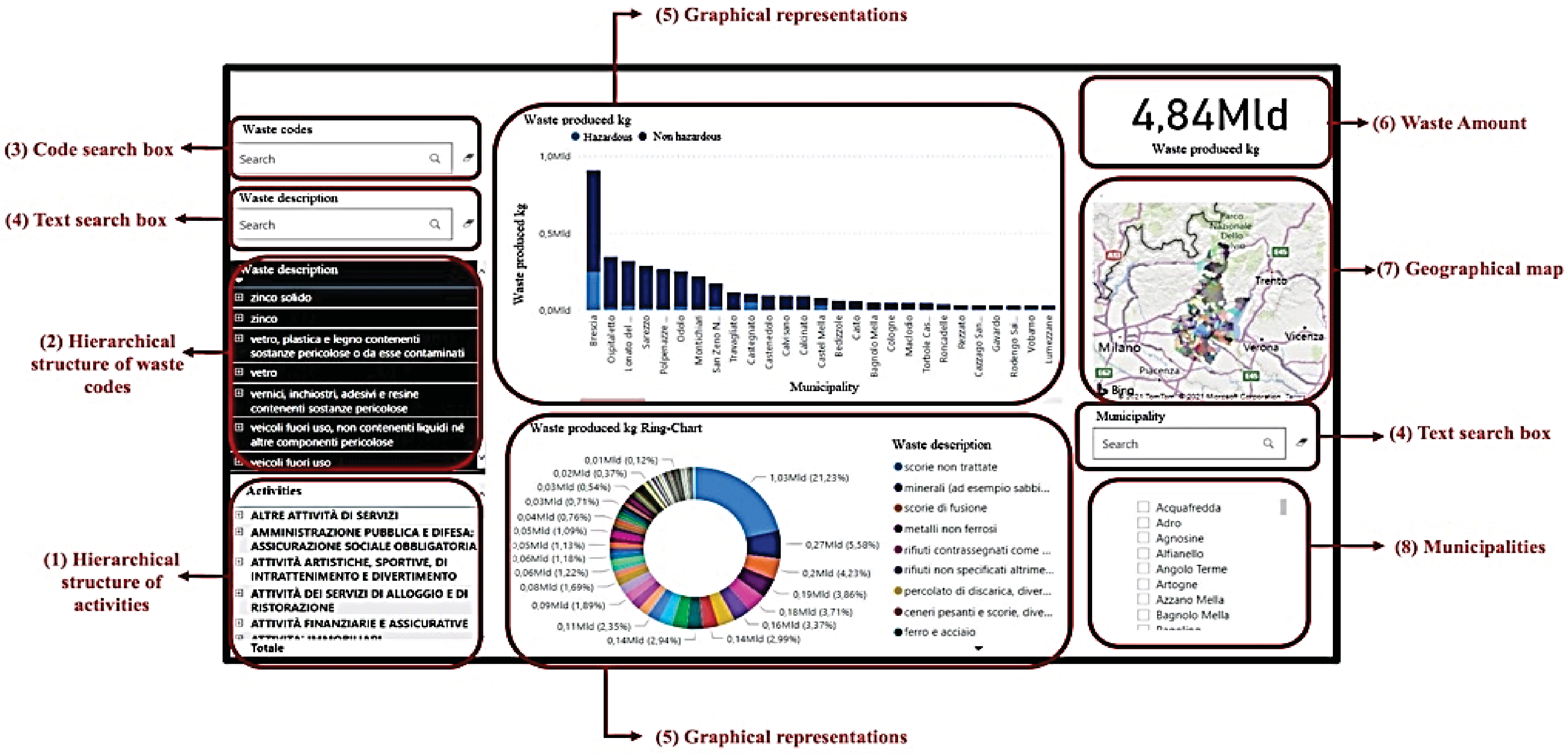


Fig. 3. The interface of the Powerbi-based tool for the analysis of WM network inside the boundaries of the province of Brescia

Validation of the proposed model was carried out following three steps. Firstly, a few specific waste streams were selected for which it was possible to get a reliable estimation for their generation based on the data about regional production or demand. For instance, considering the iron and steel production, it was possible to estimate the total generation of slags for the whole sector considering their current industrial technologies.

Regarding wastes with urban origins, such as sludge from urban sewage wastewater networks, it was possible to estimate the total generation of biological sludge by the number of inhabitants in residential areas (Rose et al., 2015; Strande et al., 2018). This way, for several cases, the numerical results obtained from the model were compared with primary evaluations in order to find the systematic errors in the software pockets.

Secondly, the results from the model were aggregated until reaching the same scale officially reported by the regional environmental agency. One of the study's objectives was to assess the current situation of the WM performance both regarding the generation of different waste codes in every single district and the treatments that those wastes received. It also became clear during the meetings with the experts of the regional environmental agencies that specific procedures were already developed for the correct interpretation of the database to obtain the relevant data for bigger aggregations. However, for smaller data fractions, it was necessary to see if the reaggregation can produce the same results.

Thirdly, in each case that the same result was not achieved, further collaboration was asked from experts of those specific sector. This opened the pathway, which includes a closer collaboration with environmental managers of single plants who gave clear descriptions of their waste types and their potential treatments and the procedure for recording relevant data. In cases that the improvement was not possible, the limitations of the approach and the requirements for further information were identified.

3. Results and discussion

The mass balance diagram for the top rank non-hazardous waste generated in the province is shown in Fig. 4. The model shows the share of material received from other regions in the total input of the system. Although the recovery parameter in this case (R_p/OUT) is smaller than the disposal, it indicates that for a significant amount of generated waste (almost 24 %), circular solutions have already been developed. Individual companies in the steel and iron sector which produced the same waste code could compare their performance to the overall performance of the relevant sector.

While for non-hazardous waste the province developed a considerable capacity in circular business models, the same diagram for hazardous waste shows little potential in recovery and respectively higher ($DR_{national} + DR_{internat.}$)/OUT (Fig. 5). A comprehensive graphical description of the material flows was also prepared for following the circulation of each waste code toward and outward the province of Brescia. The map presented in Fig. 6 shows the geographical distribution of the elements of WM network for waste code 110105*.

The details of the current WM practices in different municipalities are presented in Fig. 7. The main types of waste produced in the province were also identified in a disaggregated manner. Therefore, it would be possible to find matching scenarios for their reuse in other symbiotic relations.

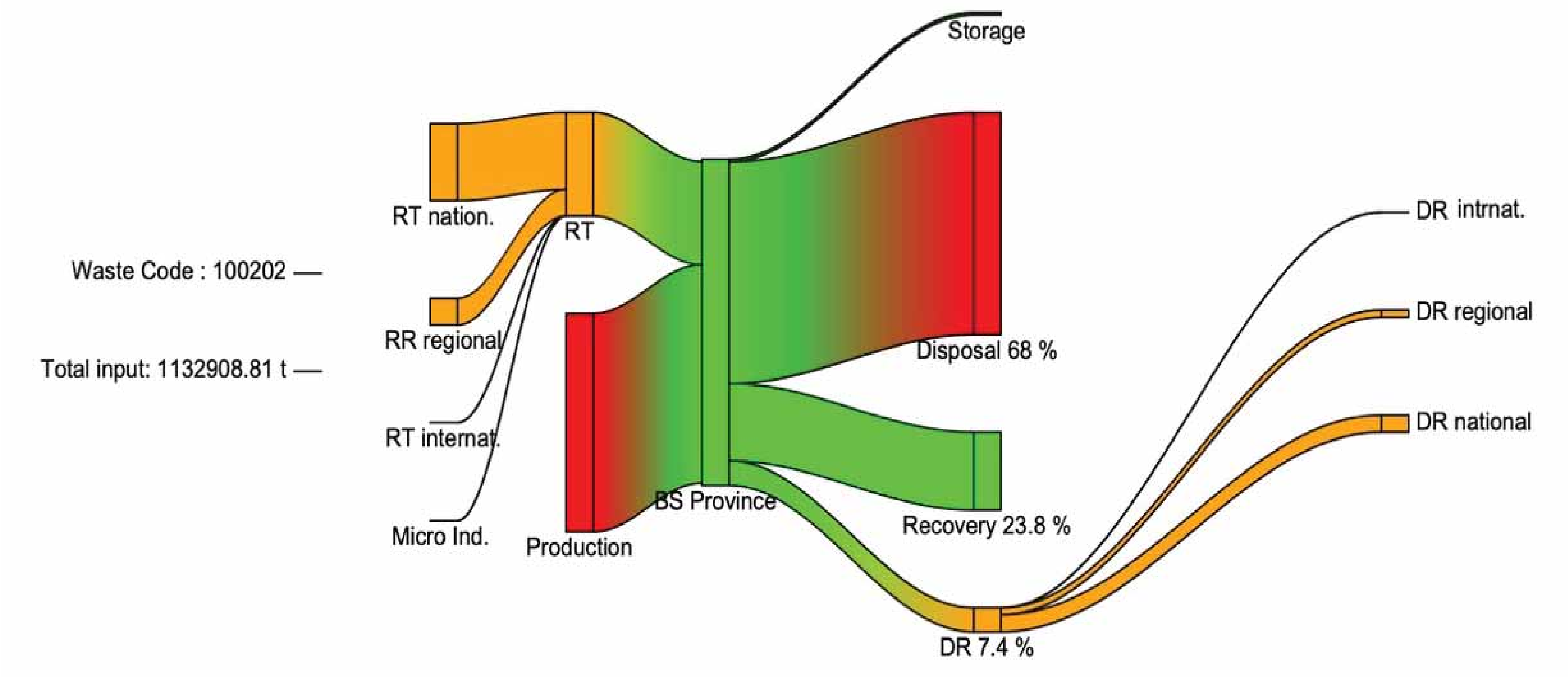


Fig. 4. Mass-balance diagram, waste recovery assessment diagram for the waste code 100202, unprocessed slags as the top rank non-hazardous waste produced in 2018 in the province of Brescia (BS)

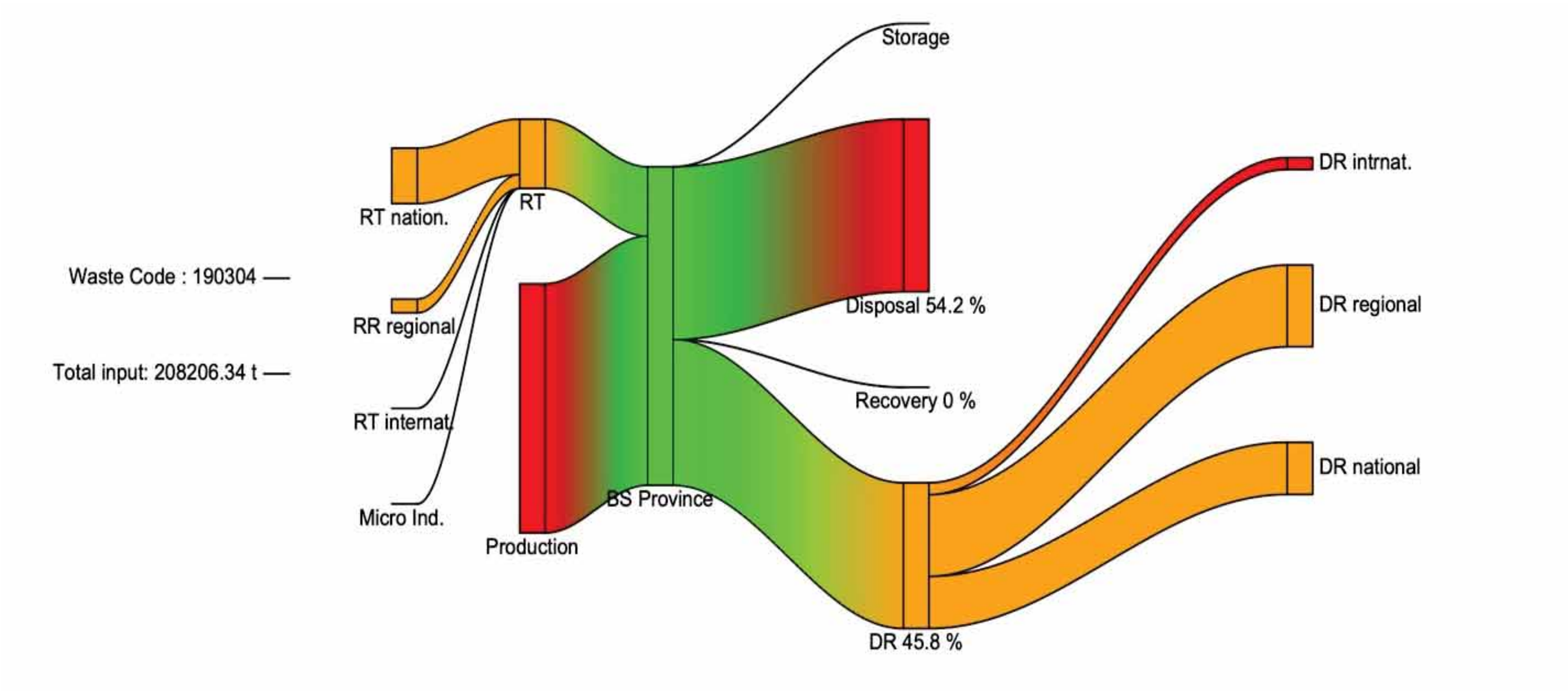


Fig. 5. Mass-balance diagram, Waste recovery assessment diagram for the waste code 190304*, as the top rank hazardous waste produced in 2018 in the province of Brescia

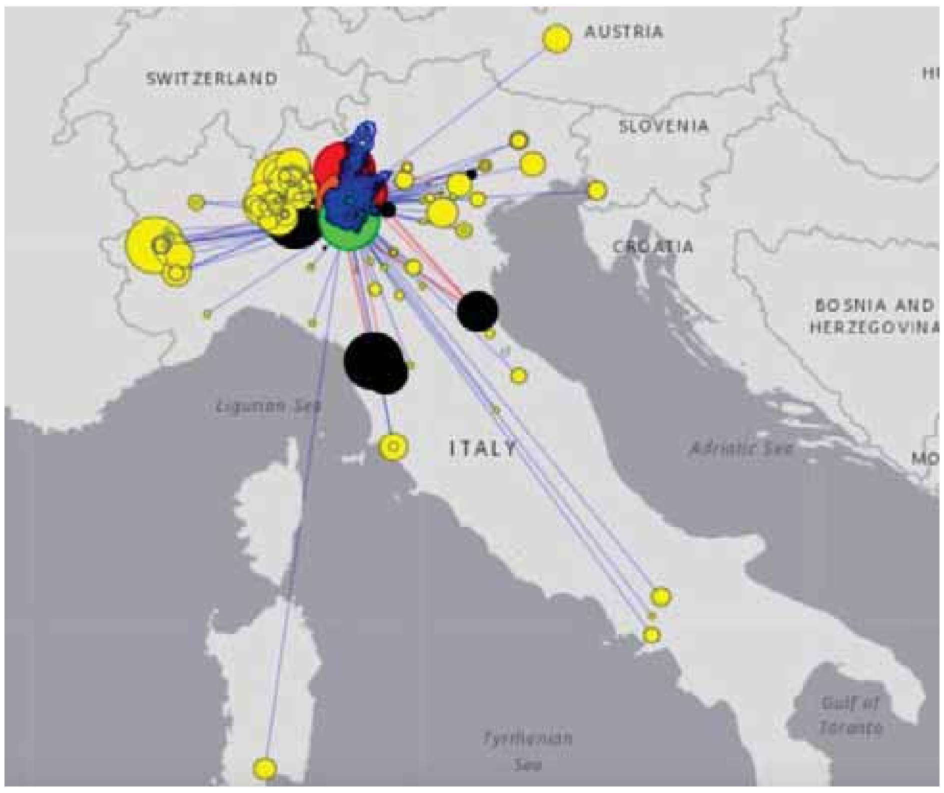


Fig. 6. Mapping the network of waste exchange for waste code 110105*

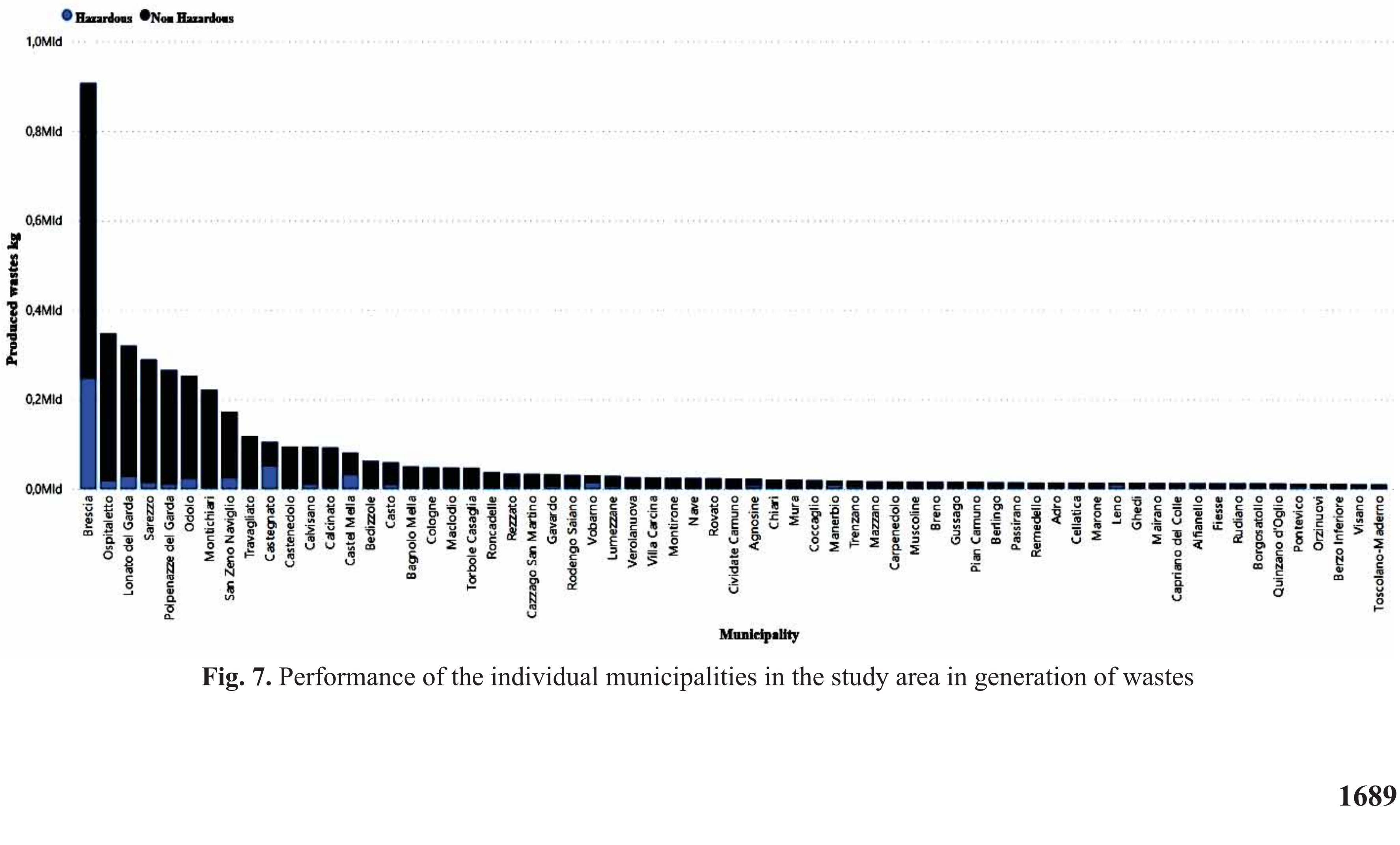


Fig. 7. Performance of the individual municipalities in the study area in generation of wastes

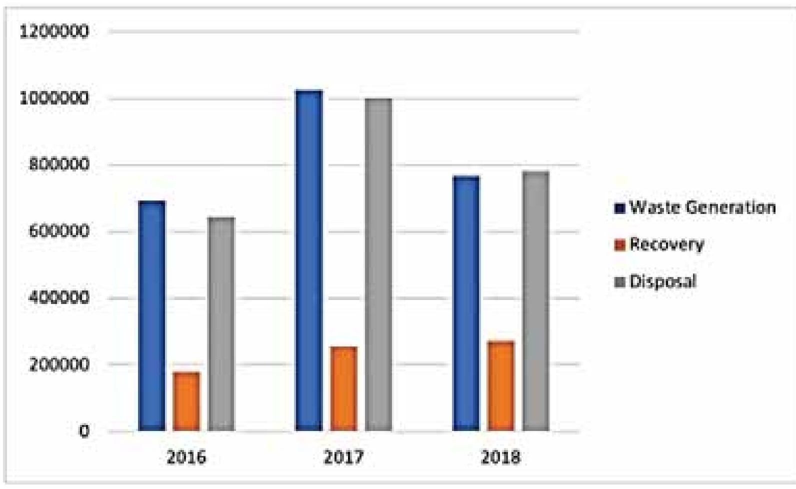
It was also found that other datasets should be integrated into the current model to make a more precise vision about the share of the companies out of the obligation for reporting waste generations, e.g., their NACE codes. Their total share in waste generation is relevant to the type of waste and may vary considerably from a code to another. However, these small firms' waste may be more suitable for recycling regarding the quality of material and purity. Therefore, the need for deepening the assessments for those industrial units is a limit of the current model even if their share has been estimated and reported as a separate group, as micro industries, based on the available information (Fig. 2).

Consideration must be made regarding some waste codes. The interpretation of the waste codes' content in terms of chemical composition and the origin of the wastes is not very simple. This is a totally different problem from the provision of verbal description for waste codes which has already been studied. For example, at present, a considerable amount of waste codes produced in the study area are those in CER families 19 and 17. However, these are mainly waste produced from secondary activities, or in other words, from the treatment of other waste codes; therefore, they may be very diverse in nature from one industrial unit to another. These groups of waste, in many cases, are landfilled or send to a farther destination for being treated. Therefore, from the environmental point of view, their recycling inside the province will result in significant benefits. However, the cost of their separation in the current situation would make it not feasible from the economic point of view. Therefore, the priority for symbiosis planning based on these results should be given to inert or non-hazardous codes and those with homogenous composition.

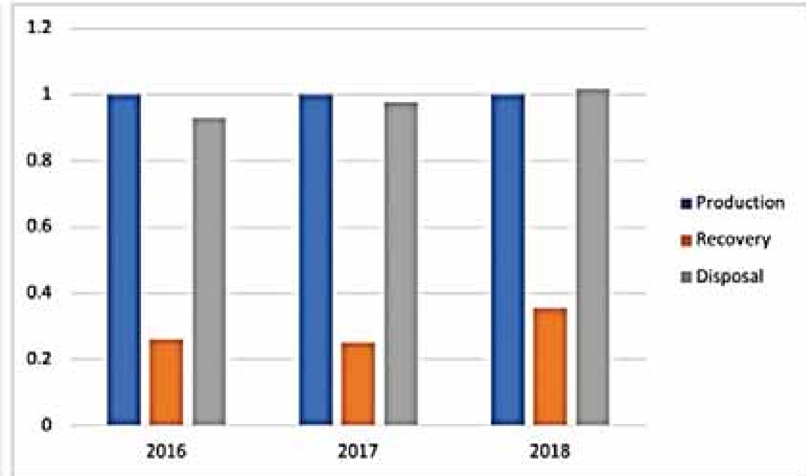
Another source of uncertainty is regarding the quantitative assessments based on annual studies. For this reason, the top-ten non-hazardous waste codes from the Powerbi-based data package were extracted and imported to the R studio mass-balance program. Comparing the performance of the study area for these waste codes in a three-year period shows little difference in the general trends of WM by normalizing the quantities for one unit of generated waste (Fig. 8b); however, the annual amount of generation and disposal may vary considerably (Fig. 8a).

This factor and the anomalies in waste amount was discussed further with the experts from the regional environmental agency and industrial experts in the province. One of the main reasons for this trend could be the entrance of unprecedented massive flows from temporary sources to the network, such as remediation activities in the ex-industrial sites. Therefore, such fluctuations in the input should be considered as a supply chain problem for CE businesses that want to consume the wastes as their principal resource.

A minimum baseline can be defined as the guaranteed amount of resource for symbiotic exchanges based on a historical study on waste generation and landfilling trends.



(a)



(b)

Fig. 8. Uncertainty analysis of WM performance for the first rank waste CER code, 100202 slags not treated, in the period 2016-2018 (a) the quantities of waste in tonnes (b) normalized situation based on one unit of waste generation

4. Conclusions

This study has provided tools for assessing WM at regional scale and parameters for evaluating CE transition by using big data analysis. The mass-balance model showed potentials for decision-making and identifying CE potentials such as industrial symbiosis by valorisation of specific waste streams to bring more effective environmental benefits to the whole system.

After removing double-counting cases and uncertainties, the output of the tools was used for assessing two parameters which already considered as relevant CE indicators, i.e., the share of the material recovery in total WM output (R_p/OUT), and the landfilling tendency (D_p/OUT) for specific waste flows and industrial sectors. The flows of non-hazardous wastes with minor recoveries ($M_p >> R_p > 0$) were also selected for conducting in-depth studies to understand the possible barriers against the expansion of CE. Moreover, using the NACE codes for aggregating the performance of similar units, it became possible to compare the circularity in the production for every single company against the overall performance of its relevant local sector.

The study area showed two main behaviours in applying CE solutions in WM. The considerably high amounts of (R_p/OUT) in managing non-hazardous wastes demonstrated promising potentials. However, the management of hazardous wastes still needs improvement since the ($DR_{national}$ + $DR_{internat.}$)/OUT and (D_p/OUT) were very high for this category.

It should also be noted that the concept of circular economy is broader than recycling, and the parameters which we reported covers partially this task. One of the important limits of this method is the uncertainty about the quality of waste streams with the same code which come from different treatment plants. Therefore, the homogeneity of waste streams needs to be evaluated and added as another indicator to the final analysis.

An essential element in the original dataset is the role of smaller companies and non-industrial entities whose generated waste enters the system. Further insights might be required for characterization of waste streams from this type of input, i.e., data provision from other sources.

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ENVIRONMENTAL IMPACTS QUANTIFICATION OF PVC PRODUCTION

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Abstract

Due to the increasing and hazardous level of plastic pollution in our planet, many researchers and experts from the public and private sector have been working in order to promote and implement solutions overcoming this global issue.
The present project joins the scientific community in this discussion by focusing on polyvinyl chloride (PVC), which is considered one of the most used polymers in engineering infrastructures. The goal of the paper is to quantitatively assess environmental impacts of the PVC production with the aim of proposing cleaner industrial solutions and more environmentally sound products.
To this end, a Life Cycle Assessment analysis was used to evaluate the environmental performance of the PVC manufacturing process. The functional unit considered was 1 kg of PVC granules. The modelling was facilitated by the Gabi software developed with three different characterization methods: CML 2001, EDIP 2003 and ReCipe 1.08. Fossil fuels depletion, climate change and human toxicity resulted to be the most significant impact categories due, respectively, to the huge quantity of crude oil extracted, the big amount of emission released into the atmosphere and the intensive toxic substances involved during the whole process.
In the last section, a number of recycling and raw material alternatives were suggested to reduce the environmental impact obtained from the analysis.

Key words: Life Cycle Assessment, Polyvinyl Chloride, PVC granules, PVC recycling

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1. Introduction

Plastic is a family of different materials. It is divided between thermoplastic that can be melted and hardened depending if it is heated or cooled and thermoset plastic that changes chemically while heated and it cannot return to its original form once melted (Plastics Europe, 2019). Polyvinyl Chloride (PVC) is a thermoplastic and it represents the third most used polymer after polyethylene and polypropylene (Elashmawi et al., 2017; Prieto et al., 2016; Rangaswamy et al., 2018). Combined with some additives, it is one of the most versatile thermoplastic polymers (Pita et al., 2002).

In 2018 the plastic production reached 359 million tons worldwide (Peng et al., 2020; PlasticEurope, 2019). This number is expected to double in the next two decades and almost quadruple by 2050 (EMAF, 2016; Samani and Meer, 2019; Venkatachalam, 2018). Out of this total amount, 61.8 million tons are produced in Europe alone, which counts for 17% of the global production (PlasticEurope, 2019). The European plastic converters demand in 2018 was 51.2 million tons, of

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which packaging and building & construction represent the main sectors. In particular, PVC constitutes 10% of the total European amount mainly for building and construction activities (Plastics Europe, 2019) and its global production also increases by 3.2% every year (CR, 2014; Peng et al., 2020).

The PVC industry is surely a significant sector since it is involved in several applications: health and safety (it is broadly used in the medical sectors); pipes construction in order to supply clean water; packaging applications; survival equipment (such as life jackets); food packaging; children's toys; bottles; cables (ECVM et al., 2000; Liu et al., 2020). It is also an important socio-economic sector since it creates multiple jobs and opportunities with remarkable incomes (ECVM et al., 2000). In Europe it comprises over 21.000 companies, creating more than 530.000 new jobs with a final turnover higher than 72 billion euros (CEC, 2000).

More specifically, in commercial terms, PVC is a widely used polymer and it is applied in both forms: rigid and flexible (Fig. 1). The first is mainly used for pipes constructions, profile applications (windows and doors), packaging, cards, while the latter is obtained by means of plasticizers and mostly used in plumbing and rubber substitution (Khaleghi et al., 2017; McKeen, 2012; Peng et al., 2020).

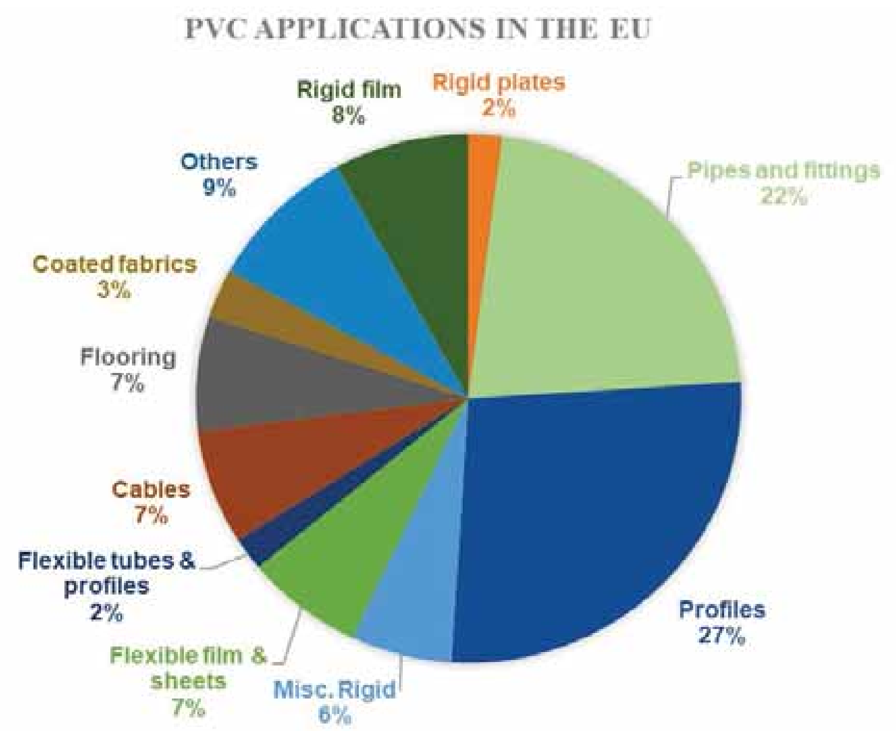

Fig. 1 PVC applications in Europe (Adapted upon ECVM, 2017)

The huge amount of PVC use leads to a large waste generation that needs to be monitored and analyzed in detail to improve end-of-life solutions (Mohammed, 2019). The challenge, hence, is to extend and turn the PVC industry into a sustainable sector. The European PVC industry keeps researching sustainability and circular economy-related projects by working on two parallel goals: to assess and improve the present situation and to develop sustainable commitments for future scenarios (ECVM et al., 2000). Moreover, the scientific communities and the private sectors are also developing overcoming solutions to reduce the polluting character of the PVC process industry (Falcke et al., 2017).

Among many, this section explores the work performed by VinylPlus, which is the 10 years Voluntary Commitment of European PVC industry towards a sustainable development (Vinyl Plus, 2017). The initiative is addressed to different scopes: reducing and/or minimizing the environmental impact during the production, promoting correct and fair use of additives, supporting waste collection and recycling alternatives, and encouraging discussion and dialogue among the PVC industry's stakeholders and decision-makers.

Given the peculiar nature of PVC, VinylPlus thereby suggests that we should dive deeper into innovative recycling alternatives for this specific type of plastic. Studies have also proven that depending on its applications, PVC can be recycled several times as, during the recycling process, the molecular chain length does not decrease (Vinyl Plus, 2017). This characteristic enables the recycled PVC to perform as well as virgin PVC.

Currently, two main methods are used for PVC recycling: mechanical recycling and feedstock recycling. Mechanical recycling is the process through which no polymer chains are broken down into smaller particles but rather, the components are mechanically separated and sorted into smaller fractions. It is divided into two categories: conventional and non-conventional technologies. The conventional technologies consist of sorting, shredding, and separating particles to obtain in the end a pulverized/granulated recycled PVC; on the other hand, non-conventional technologies make use of solvent-based processes and it generally suits better more complicated waste streams. The other option is feedstock recycling. The feedstock recycling process consists of the thermal treatment of the PVC waste and in most cases the hydrogen chloride is recovered and it can be sent back to the PVC production or it can be used in other applications (Vinyl Plus, 2020).

In 2019 VinylPlus reached 771,313 tonnes of PVC waste recycled, 4.3 % more compared to 2018, saving 1.5 million tonnes of CO_2 (VinylPlus Report, 2020). Within the EU Circular Plastic Alliance (CPA), VinylPlus committed to boosting its recycling rate up to 900,000 tonnes of PVC by 2025 and to at least one million tonnes by 2030 (VinylPlus Report, 2020).

Many research projects demonstrated the excellent performance of PVC recycling and the related environmental benefits. For instance, previous LCA-based studies have proved the importance of replacing raw materials to reduce potential PVC environmental impacts (Comanita et al., 2015; PlasticEurope, 2008). More specifically, according to Alsabri et al. (2020), in the piping industry, a switch to recycled polyvinyl chloride can reduce the climate impact from 36.21% to 15.53% for the production of 1 ton of polyvinyl chloride. Whereas, by analyzing the life cycle of PVC windows frame on both post-industrial and post-consumer waste, it was demonstrated that replacing virgin PVC with PVC from post – consumer waste saves around 2 tons of CO_2 eq./t while replacing virgin PVC from post-industrial waste saves around 1.8 tonnes of CO_2 eq./t (Stichnothe and Azapagic, 2012).

This study joins the scientific community by analyzing, specifically, the full life cycle of the PVC industrial life. The paper is divided into different sections: it starts with an extended overview of the PVC characterization and industry together with an LCA approach model in the materials and methods sections. The results of the assessment are then discussed. Finally, a review of current and more sustainable alternatives is reported.

2. Material and methods

2.1. PVC characterization

PVC is a chlorinated hydrocarbon polymer. The carbon atoms in the main chains are alternatively linked to hydrogen atoms and chlorine atoms. PVC is the result of the chemical polymerization of the vinyl chloride during which the double bond molecule is broken down to form a longer chain polymer (Fig. 2, Boustead, 2005). The production of PVC involves three main stages: the upstream of the PVC industry, the PVC industry, and the downstream of the PVC industry (Fig. 3).

The raw materials for the production of PVC are ethylene and chlorine, which are supplied upstream by the petrochemical industry (for ethylene) and the soda industry (for chlorine) (Pascault et al., 2012). The petrochemical industry produces ethylene through thermal cracking of naphtha, while the soda industry generates caustic soda, chlorine, and hydrogen thanks to electrolysis. Using ethylene and chlorine the PVC industry is able to manufacture an intermediate material called EDC which will thermally be cracked into VCM that eventually is polymerized to obtain PVC. In the downstream industry, PVC is mixed with several additives, stabilizers, and plasticizers (VEC, 2008).

Additives are necessary to guarantee specific properties to the final PVC product and they vary according to the intended application. Stabilisers are the ones that need to be assessed more carefully due to their hazardous features and, thus, their potential dangerousness for human health. They are added to help the PVC polymer not to degrade (Guangbao, 2020). The most used ones are lead stabilizers and cadmium stabilizers (CEC, 2000). On the other hand, plasticisers are added in order to obtain flexibility and workability in PVC products (Pereira et al., 2019). Also, in this case, the quantities of the plasticisers change according to the desired properties and the final use (CEC, 2000).

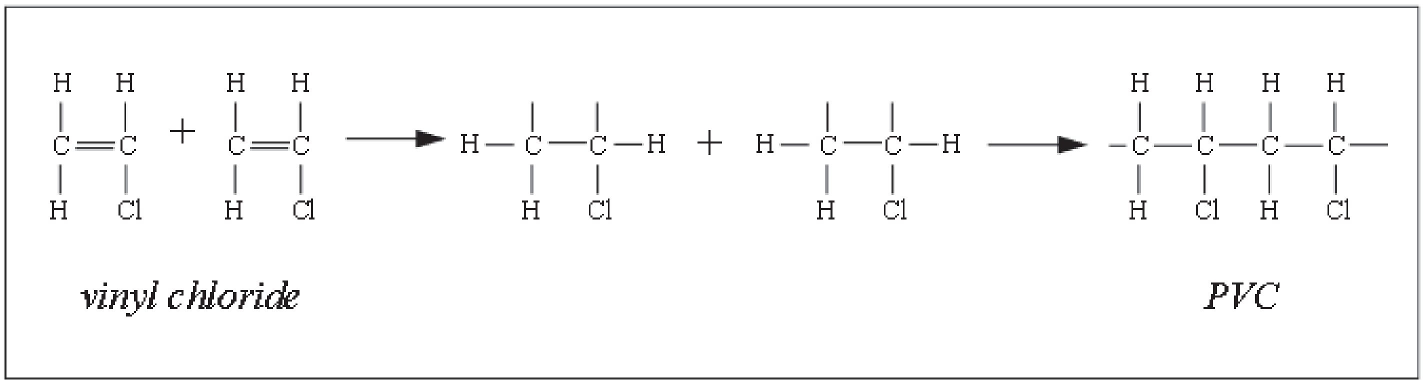

Fig. 2. Schematic representation of the polymerization of vinyl chloride (Boustead, 2005)

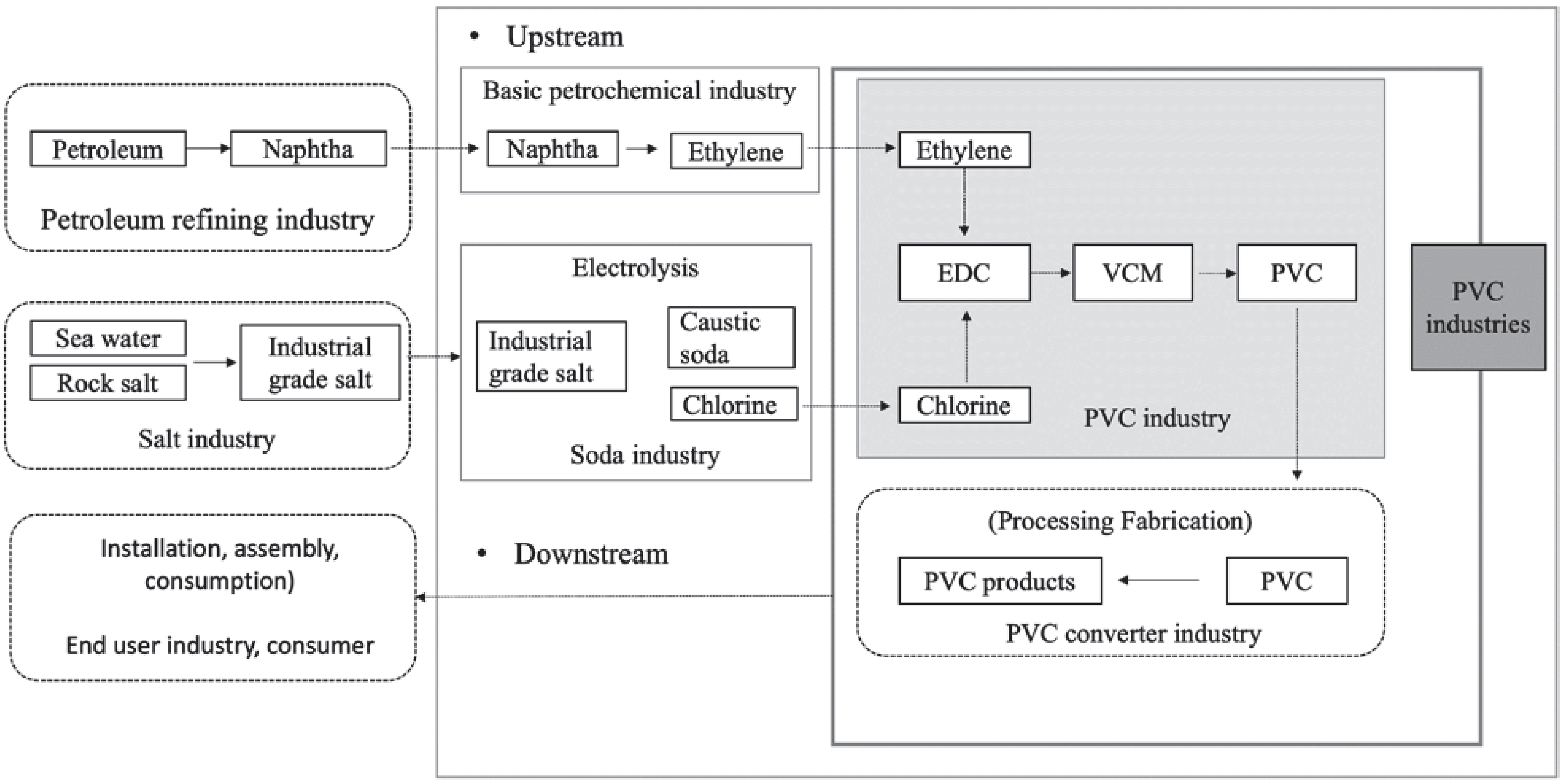

Fig. 3. Linkage of PVC related industries (Adapted upon VEC, 2008)

2.2. Methodology

The methodology adopted in this study is Life Cycle Assessment (LCA), which is an iterative tool able to identify possible environmental impacts associated with products and/or services (ISO 14040, 2006). According to the ISO 14040/44 four iterative stages are necessary in order to perform a valid LCA (ISO 14040, 2006; ISO 14044, 2006; Megange et al., 2020), as shown in Fig. 4.

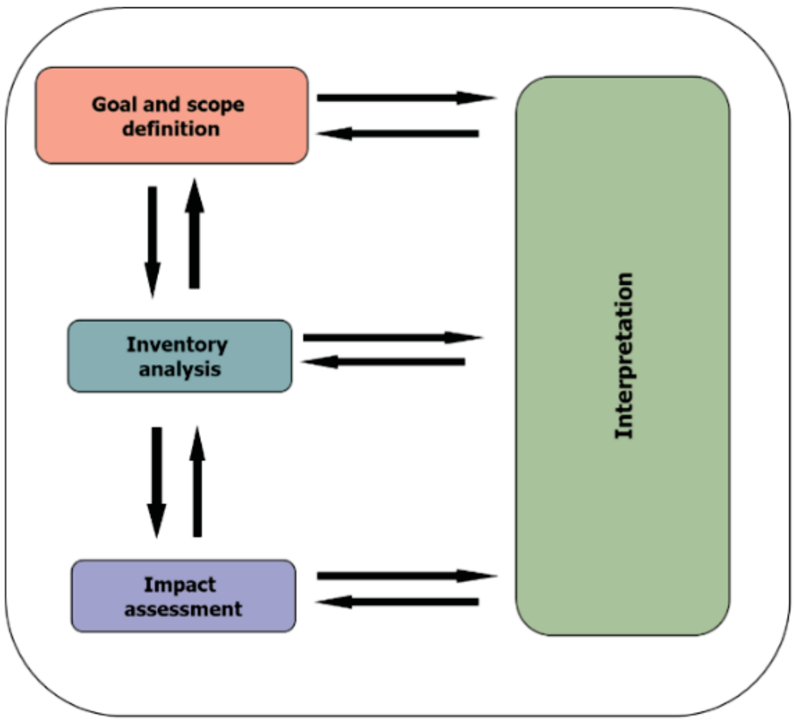

Fig. 4. Framework of LCA modified from the ISO 14040 standard (Hauschild et al., 2018)

2.3. Goal and scope definition

LCA has been performed in order to develop a quantitative analysis of the environmental impacts generated during the life cycle of a PVC product. The functional unit is 1 kg of Polyvinyl Chloride granules (raw material which eventually will be processed into final products). Data included in the study were gathered from literature and adapted to 1 kg of PVC considered (Boustead, 2005; Comanita et al., 2015; Ghinea, 2015; PlasticsEurope 2018). Additionally, missing data have been found in the Gabi database according to the purpose of the study.

The analysis focuses on the boundaries *cradle to gate* including all the stages from the raw materials extraction up to the end of the manufacturing industry. All the phases concerning the distribution, the use and the end of life have not been taken into consideration as they are not particularly relevant for the scope of the analysis. The methodologies chosen to run the LCIA are: ReCipe 1.08, EDIP 2003 and CML 2001. The results obtained are presented in normalized values-EU 25+3.

2.4. Life Cycle Inventory (LCI)

The inventory model is a crucial step in the LCA analysis as it links all unit processes involved in the study until the final product (Hauschild et al., 2018). This phase aims to collect all necessary quantities to develop product/waste flows and elementary flows dividing them between inputs and outputs within the system boundaries selected (Fig. 5). The inputs consist of the materials, energy and resources that enter into the unit process, whereas the outputs are represented by the products, waste and emissions resulting from the process (Hauschild et al., 2018). The inventory model of the analyzed PVC production has been developed dividing the system in three main stages of the life cycle process. Table 1 represents the LCI referred to 1 kg of polyvinyl chloride from suspension polymerization (S-PVC).

Particularly, a foreground system (consisting of the dataset strictly related to the study analyzed) are literature data adapted to the study purposes (Boustead, 2005; Comanita et al., 2016b; PlasticsEurope, 2019). Whereas, the background dataset consists of secondary data gathered in the Gabi software.

Table. 1. Life Cycle Inventory

I STEP: Ethane (C2H4) and Chlorine (Cl2) Production	
Input	***[kg]***
Petroleum	53.7
Salt (NaCl)	0.0015
Output	[kg]
Dioxins	0.0044
Particulates < 10µm	0.0035
Chlorides suspension	0.0003
NMVOC	0.0022
NaOH	0.0025
Cl_2 (chlorine)	0.0088
C_2H_4 (ethane)	0.9538
II STEP: VCM production process	
Input	***[kg]***
C_2H_4 (ethane)	0.9538
Cl_2	0.0088
H2	0.0783
$CuCl_2$	0.0044
O_2	0.0074
EDC impure	0.0845
EDC pure	0.3978
HCl	0.0349

Bentonite	0.0492
Distillation water	1.0280
Organic peroxides	0.0197
VCM impure	0.0857
VCM pure	0.0893
Output Materials	***[kg]***
Chlorinated hydrocarbons	0.0024
CO	0.0025
CO_2	0.0146
Waste water	0.631
NMVOC	0.001
NOx	0.0001
Energy released in the exothermal process - Output	**[kJ]**
Energy	0.027
III STEP: PVC production process	
Input Materials	***[kg]***
VCM pure	0.0893
Phenol	0.0013
Ca stabilizer	0.0023
Hydroxide	0.0002
Methylamine	0.0298
1,4-Butanediol	0.0023
2-methyl-2-butene	0.0027
Water	2.2390
Energy - Input	**[kJ]**
Energy	0.1509
Output Materials	***[kg]***
NMVOC	0.0016
Waste water	1.8328
PAH	0.0239
COD	0.0024
TOC	0.0073
Particulates < 10 ppm	0.003
PVC susp. from polymerization	1.0359
PVC from omogenization	1.9380
PVC from centrifugation	1.8370
PVC from washing	2.8390
Pure PVC from drying	1.0000

2.5. Life Cycle Impact Assessment (LCIA)

The third phase of the LCA is the Life Cycle Impact Assessment, during which the elementary flow resulting from the LCI are translated into environmental impacts (Hauschild et al., 2018). According to the ISO 14040, (2006) and ISO 14044 (2006) three steps are mandatory in a LCA analysis: the selection of a characterization model, the classification step and the characterization. As far as the first step is concerned, different characterization methods exist and they generally consist of two approaches: the problem-oriented approach called *mid – point* and the damage-oriented approach called *end-point*.

This study considers three different methodologies in order to propose a comparison between the results obtained. The characterization models chosen are: ReCiPe 1.08 (end-point), EDIP 2003 (mid-point) and CML 2001 (mid-point).

The indicators considered from the **ReCiPe 1.08** model are: *agricultural land occupation (ALO), climate change ecosystem (CCE), climate change human health (CCHH), fossil depletion (FD), freshwater ecotoxicity (FEc), freshwater eutrophication (Feu), human toxicity (HT), marine ecotoxicity (ME), metal depletion (MD), natural land transformation (NLT), ozone depletion (OD), particulate matter formation (PMF), photochemical oxidant formation (POF), terrestrial acidification (TA), terrestrial ecotoxicity (TE), urban land occupation (ULO).*

The second impact assessment methodology applied is **EDIP 2003**, which covers the following indicators: *acidification potential (AP), global warming (GW), photochemical ozone formation (POF) with impacts both on human health and vegetation, terrestrial eutrophication (TE) and aquatic eutrophication (AE)*

The last characterization model chosen is **CML 2001**, which focuses on the following impact categories: *Abiotic Depletion (ADP), Abiotic Depletion (ADP fossil), Acidification Potential (AP), Eutrophication Potential (EP), Freshwater Aquatic Ecotoxicity Pot. (FAETP), Global Warming Potential (GWP), Human Toxicity Potential (HTP), Marine Aquatic Ecotoxicity Pot. (MAETP), Ozone Layer Depletion Potential (ODP), Photochemical Ozone Creation Potential (POCP), Terrestrial Ecotoxicity Potential (TETP).*

3. Results and discussion

This section will, firstly, describe the results obtained through the three different methodologies and, then, it will give a little discussion over the PVC industry by suggesting potential solutions for its polluting nature.

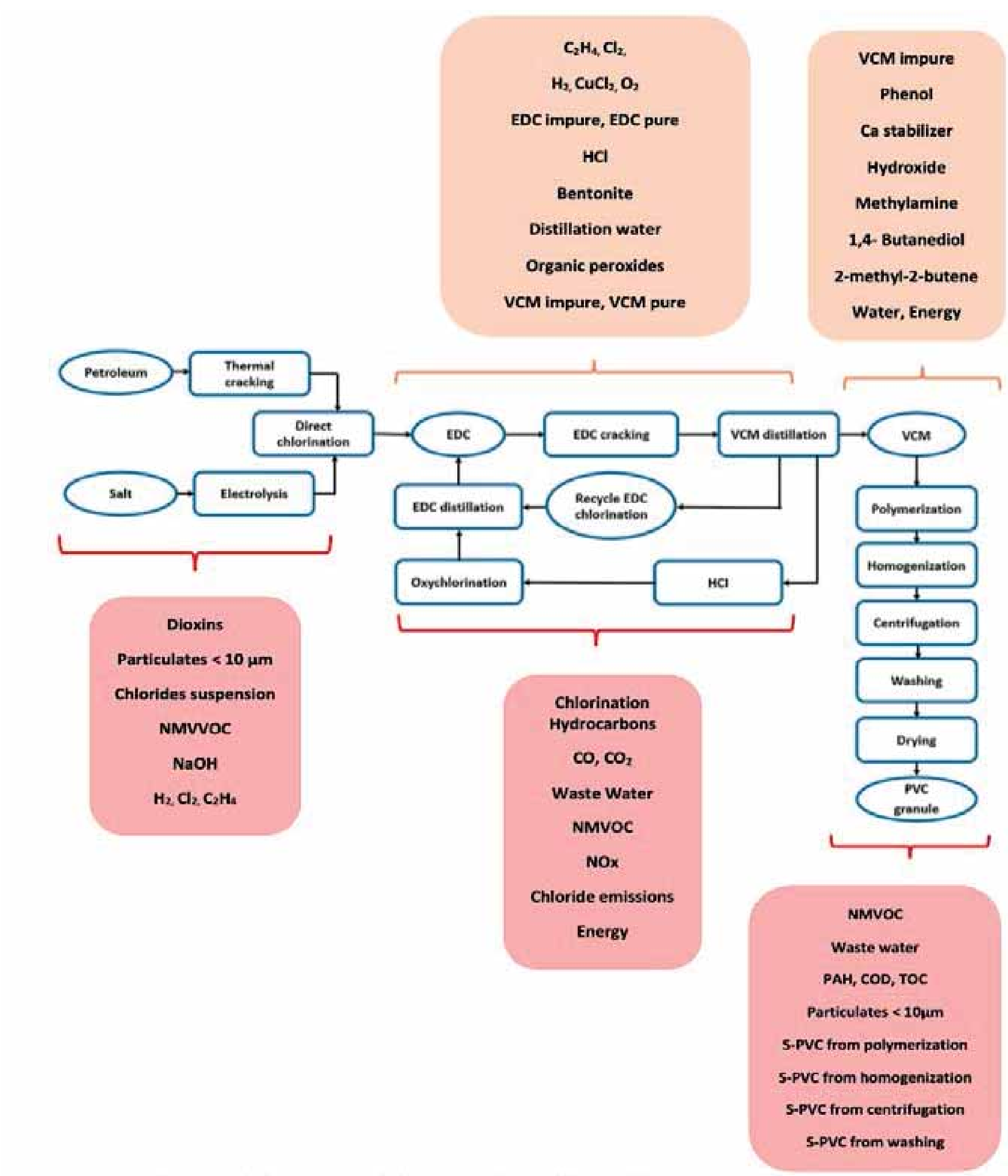

Fig. 5. Life cycle inventory (adapted upon Comanita et al., 2016a)

3.1. Environmental impact assessment with ReCiPe 1.08 methodology

The main environmental impacts resulting from the ReCiPe 1.08 methodology are shown in Fig.6, which are expressed in equivalent per person. The four categories are represented by a positive value, which means that they generate negative impacts on the environment.

According to the obtained results, *Fossil Depletion* (FD) shows the highest environmental impact, which is likely due to the large amount of crude oil extracted for the production of 1 kg of PVC; the second relevant impact category *Human Toxicity* (HT) is caused by the significant amount of hazardous and toxic substances used during the PVC processing production. The third biggest contribution is given by Climate Change. ReCiPe, in particular, considers human health damage (CCH) and loss of species (CCE): the characterization factor of human health damage is expressed in DALY, while the loss of species is calculated in Potential Disappeared Fraction of species (PDF) (ILCD Handbook, 2010a). Regarding the impacts generated by the consumption of chemicals, it was found that NO_2 and NO emissions are generated as a result of the use of catalysts for obtaining ethene. This leads to negative impacts associated with climate change, damaging both the ecosystem and human health.

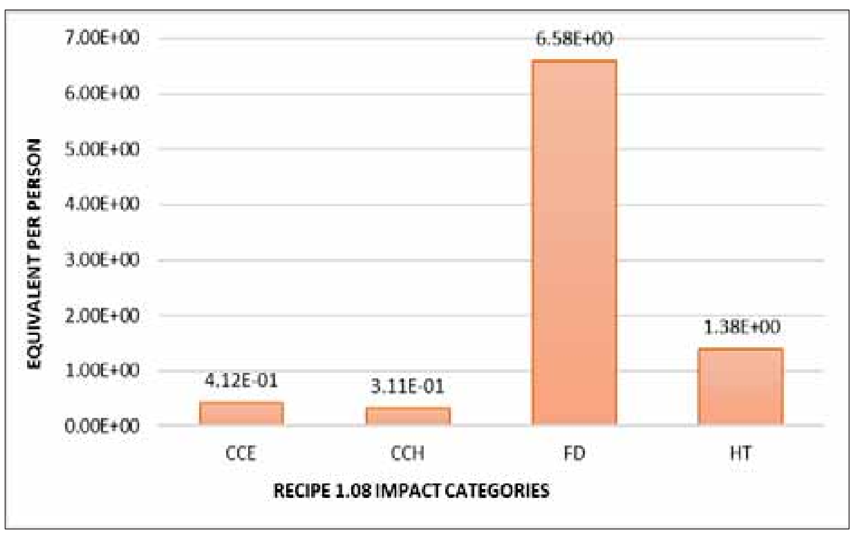

Fig. 6. ReCiPe 1.08 methodology - environmental impacts of PVC production

3.2. Environmental impact assessment with EDIP 2003 methodology

Fig. 7 represents the main impact categories obtained by applying the EDIP 2003 methodology. In this case, the *Global Warming Potential* has the highest value followed by the *Photochemical Ozone Formation* applied on two subcategories. The first is *Photochemical Ozone Formation human health,* which is modelled in line with the number of people extra exposed according to the WHO guide (WHO, 1989) for chronic effects time duration, expressed in pers·ppm·hours; the second is *Photochemical Ozone Formation vegetation,* which is identified as a specific ecosystem area overexposed for chronic effects time duration compared to the threshold given by WHO expressed in m^2·ppm·hours (ILCD Handbook, 2010b; 2011). Minor impacts are given by acidification potential, aquatic eutrophication, and terrestrial eutrophication. The presence of catalysts used for obtaining vinyl monomer has a significant contribution to the *Global Warming Potential*.

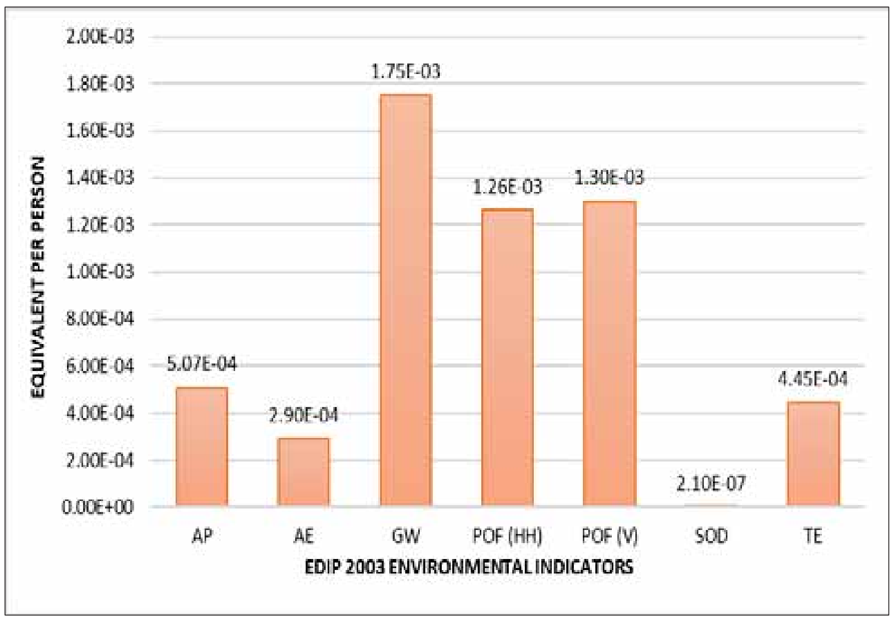

Fig. 7. EDIP 2003 methodology environmental impacts of PVC production

3.3. Environmental impact assessment with CML 2001 methodology

In this case, even if all impact categories shown in Fig. 8 have a positive value, they are quite small. Smaller contributions are given by: *Abiotic Depletion* (ADP), *Freshwater Aquatic Ecotoxicity* (FAE), *Marine Aquatic Ecotoxicity* (MAE), and *Terrestrial Ecotoxicity Potential* (TETP). The high values of FAE and MAE are given by the high content of nitrogen and phosphorus resulting from additives added in the polymerization process.

The outcoming scenario shows that the PVC life cycle analyzed (from the extraction of the raw materials until the end of the production) is environmentally harmful due to many polluting actors involved throughout the whole process. Figure 8 shows, for instance, a comparison of the impact assessment on human health between the ReCiPe and CML models. Chemicals (phthalates, ethylene, stabilizers, pigments) used in the production of PVC release emissions into the environment that have a negative impact on human health. Also, the process of obtaining PVC induces negative effects in the environment associated with the impact category of human health (Fig. 9). The generation of this type of impact is the consequence of chlorine emissions from the electrolysis stage of sodium chloride.

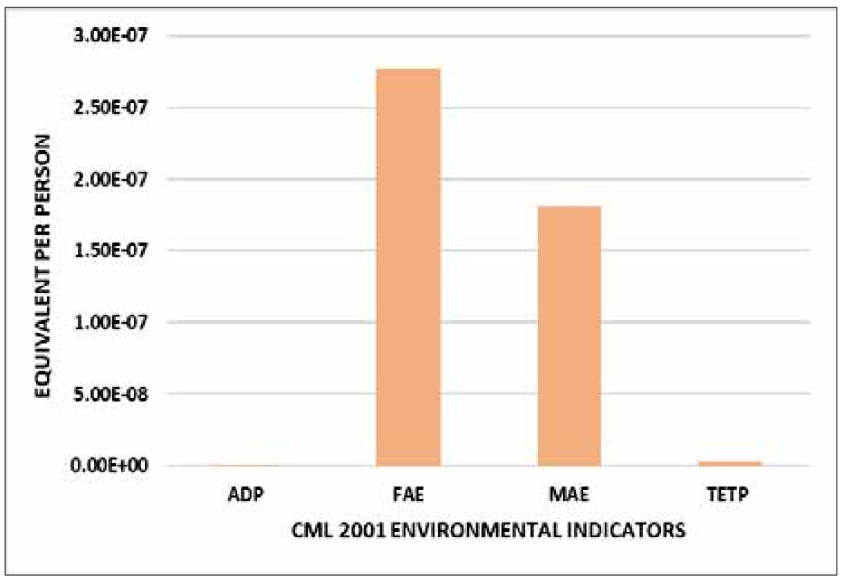

Fig. 8. CML 2001 methodology - environmental impacts of PVC production

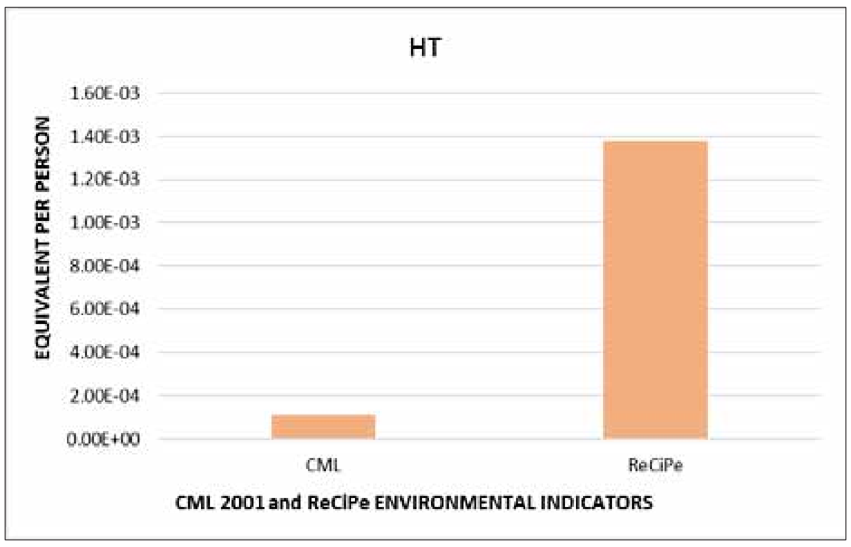

Fig. 9. Comparative evaluation of the impact on human health - ReCiPe vs CML

3.4. Suggestions for virgin PVC replacement

The results confirmed the big issue represented by the use of harmful feedstock in the plastic industry. Raw materials were a crucial topic ever since the very beginning of plastic; it was proved that more than 95% of the plastic present worldwide is fossil-based plastic (Plastics Europe, 2018).

In spite of this, innovation and research have started to undertake a very clear direction by boosting sustainability at its maximum rate and creating more environmentally sound solutions for today's global issues (Fortuna et al., 2012). Within the current circular economy perspective, also plastic has found a new way to reshape itself. One of the possible alternatives to fossil-based plastic is *bioplastics*. Bioplastics are that plastic that are either bio-based, biodegradable, or both (Europe Bioplastics, 2018).

Bio-based refers to the origin of the material, meaning that the raw material comes fully or partially from biomass, whereas biodegradable refers to the end of life of the plastic product. Biodegradable plastic is one able to chemically degrade itself thanks to microorganisms that turn the materials into water, carbon oxide, or compost (Europe Bioplastics, 2018).

Not all bioplastics are biodegradable and vice-versa. More specifically, according to Europe Bioplastics, bioplastics are divided in three categories: the first are those fully or partially bio-based but not biodegradable such as bio-based PE, PP, or PET, PA, PTT (mainly called drop-ins); the second type are both bio-based and biodegradable PHA, PLA and PBS; and finally, biodegradable fossil-based plastic such as PBAT (Europe Bioplastics, 2018).

Bioplastics do not even represent one percent of the total plastic on the market today albeit their production is getting wider (Jeremic et al., 2020). In particular, almost half of bioplastics present in the market are bio-based non-biodegradable (Fig. 10).

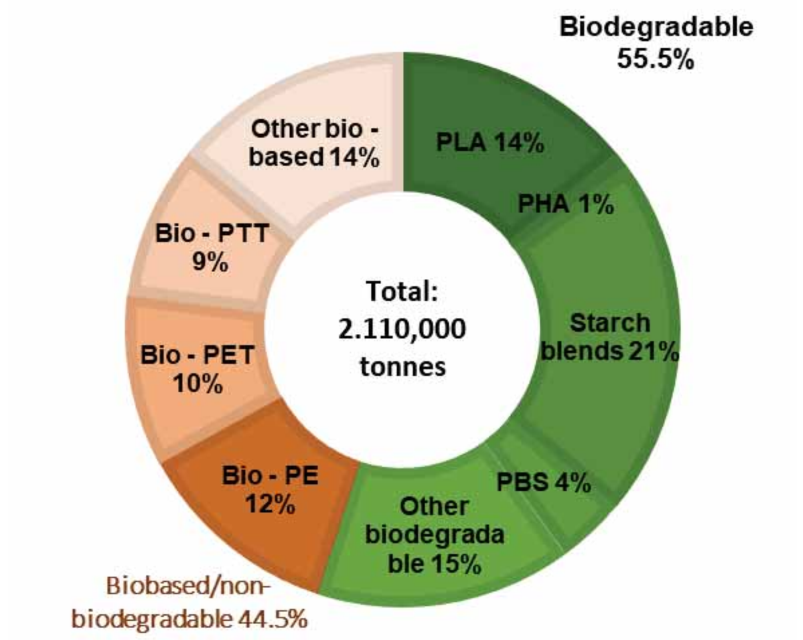

Fig. 10. Global production capacities of bio- plastics in 2019 (adapted upon Jeremic et al., 2020)

PCV can also derive from renewable feedstock and bio-PVC is expected soon to be produced boundlessly. When it comes to plastic manufacturing, plasticizers are definitely a critical issue. Particularly, in PVC production, 75% of the plasticizers used are phthalate plasticizers which are fossil-based substances (Feng et al., 2018). To overcome this, new studies and researches started to focus on developing bio-based plasticizers, which, generally, come from agricultural waste and by-products (Feng et al., 2018). The research is still open and keen to upscale bio-plasticizers to perform as well as petroleum-based plasticizers.

Obviously, bioplastics have several advantages. They contribute to resource-saving in input and to reduce GHG emissions and the overall carbon footprint of products in output (European Bioplastics, 2018). However, bioplastics are not the solution in absolute terms, and they need to be properly managed. They may become an issue in the end-of-life management; thus, it is of paramount importance to address clean and correct waste management in order to lower any potential environmental and human-related damage that they might cause. Bioplastics are able to biodegrade only in specific controlled conditions, and, consequently, they represent a serious problem if discharged erroneously (Ghinea et al., 2016; RameshKumar et al., 2020). The recycling option is considered to be the preferred solution for bioplastic. Recycling can be performed mechanically, chemically, or organically according to the most favorable condition and the composition of the specific plastic product (RameshKumar et al., 2020).

The life cycle assessment methodology, once again, represents a great tool, since it is able to analyze and assess the impacts related to bioplastic-based products throughout their entire life cycle. The paper thereupon invites to perform additional LCA-based analyses aimed at comparing the environmental performances between bio-PVC products and virgin PVC products.

5. Conclusions

This paper focuses on a specific kind of plastic which is Polyvinyl Chloride (PVC). The PVC production involves several steps and processes: raw material extraction, different sub-steps to produce EDC, and VCM and, lastly, the PVC manufacturing to obtain the final product.

In order to evaluate the environmental impacts related to the PVC industry, a Cradle-to-Gate analysis has been performed with the support of the GaBi software and the use of three characterization methods (ReCiPe 1.0, EDIP 2003, and CML 2001).

According to ReCipPe 1.08, fossil depletion is the most significant indicator, due to the fact that a huge amount of crude oil is involved in the extraction process. EDIP 2003 shows that climate change is the biggest contributor and it is related to a large number of emissions released into the environment during the production and the extraction phases. Lastly, as far as CML 2001 is concerned, in accordance with ReCiPe 1.08, human toxicity is an endangered impact category because of several toxic substances involved in the whole process.

The final part describes one of the most valid alternatives able to partially fix the environmental issue related to the PVC industry: the substitution of the raw material. Bioplastic solution is a strong option to take into consideration; past studies provided quantitative information about its efficiency and advantages. However, researching for new innovative alternatives and improving the already existing ones is an energy-demanding and time-consuming procedure. Nevertheless, there is considerable room for improvement. Therefore, this project encourages the public and the private sector to work deeper in order to change direction and reverse the current damaging trend.

This study helps to understand the major impacts that just a kilogram of PVC might have. Consequently, the study highlights the urgent need to shift direction and invest in more environmentally sound solutions in PVC production.

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ENTOSIM, AN INSECTS LIFE CYCLE SIMULATOR ENCLOSING MULTIPLE MODELS IN A DOCKER CONTAINER

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Abstract

EntoSim is a software aimed to collect different physiologically based models describing the life cycle of ectotherms and, more specifically, of insect pests. It is developed in an open-source framework including the ROOT's software libraries in a C/C++ programming language, with the purpose of an easy diffusion and compatibility. *EntoSim* could be used in model development and validation and in decision making frameworks, to support farmers and technicians to formulate low-impact control strategies. The growing availability, in literature, of physiologically based models and their utilisation in plant protection, led to explore the latest computer technologies that could be applied in entomology. This led to a significant revision of the *EntoSim* philosophy and structure. This work, therefore, aims to describe this conceptual and operational change, and its implications on *EntoSim* in order to: *i)* increase the number of options available to the users, *ii)* simplify the software development and *iii)* increase software dissemination and adoption. These three points led to the addition of two more population density models within *EntoSim*, and to the creation of the first Docker image available in a public repository for entomological purposes, to make its deployment faster. In this regard, the code structure was reorganised in modules corresponding to each *EntoSim* function; the graphical part was developed and implemented using Python language so that results are visualized directly in a web browser page. All the *EntoSim* dependencies were included into a Docker image, using Linux CentOS as base operating system.

Key words: decision support systems, descriptive models, growth models, integrated pest management, population modelling

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1. Introduction

Understanding biological phenomena is surely one of the greatest challenges of the modern times, and among the developments succeeded towards the years, mathematical modelling has always had an important role. In the fields of Agriculture, Forest and Ecological Sciences, for example, mathematical models aroused the interest of researchers since their suitability to describe phenomena, and to be used as Decision Support Systems (DSS) (Capinera, 2001; Rossini et al., 2020e; Tang and Cheke, 2008). More specifically, if a mathematical model faithfully represents a particular phenomenon, such as pests outbreaks, it could provide a prediction of the risks of future infestations, on the basis of the past and present data (Sinclair and Seligman, 1996). The main reason to invest human and economic resources on the development of mathematical models is their role in the reduction of the inputs (such as pesticides or agrochemicals) in the cultivated fields, with a subsequent increase of the biodiversity and of the environmental health (Bange et al., 2004; Knight and Mumford, 1994).

To protect plants from insect pest infestations, several mathematical models were developed applying different theories and hypotheses (Orlandini et al., 2018), but their common point is the use of computational tools providing numerical solutions and parameters from experimental data (Holst, 2013). Generally speaking, an ideal application of a mathematical model in pest population description is

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composed by three "macro-steps" (Bellocchi et al., 2011; Rossini et al., 2019a, 2019b): *i)* a laboratory phase, where parameters specific for the species are estimated with experimental data; *ii)* a simulation phase, where the parameters of the previous phase and environmental data are inserted into the population density model, subsequently solved numerically; *iii)* a validation phase, where simulations are compared with data collected *ad hoc* in an experimental field.

To date there are several software programs which may support the operations reported so far, but most of them need an adaptation or a license. A recent work by Rossini et al. (2019a) discussed the possibility to use ROOT (Brun and Rademakers, 1997), an open source software developed for high energy physics data analysis, to support the model application in entomology. More specifically, ROOT's libraries are particularly suitable for the fitting operations, which lead to the estimation of the model parameters in the so called "laboratory phase", and to graphically represent the results. In their initial idea, the description of a series of macros, corresponding to each step of a model application, was provided, showing a great potential in terms of versatility (Rossini et al., 2020d) and reduction of software costs.

However, biological and mathematical modelling are part of a greater field of data analysis which is constantly trying to solve problems of results reproducibility, software and scripts compatibility among different operating systems or software licence requirements. Moreover, this growing field of science needs highly skilled users that not all the research groups are equipped with. This aspect is particularly highlighted by the increasing availability of data, software and scripts provided as supporting information with the scientific articles.

Recently, scientist's attention has been captured by Docker, an open-source project developed with the aim of deliver pre-assembled packages called image containers, that will be run in a virtualization mode (Docker, 2021). Thus, it is possible to build a Docker image container running a basic operating system and already containing all the dependencies required by the software that the developers are going to share. Furthermore, along with the software, the datasets necessary for the analyses could be also provided, so that anyone can use them to reproduce the same results, even without advanced programming skills.

Users can then easily download and use right away this virtual container, without encountering all the problems of incompatibility and reproducibility, as discussed by Di Tommaso et al. (2015) and Boettiger (2015). Furthermore, Docker is even more appealing for scientists because: *i)* it is less memory and hardware consuming than a virtual machine, and *ii)* it is also less time consuming because most of the dependencies and installation operations are already done by the developers.

Given this precondition, the main focus of this work was to improve and share *EntoSim* among model scientists who work with ectotherms, providing the community of users with the latest code and model structure modifications in a simple deployable computing environment. More specifically, the first major change was the creation of a Docker image, where *EntoSim* has been stored with all its dependencies, which can be easily "pulled" from a public repository and executed as a stand-alone Docker container. In the best of our knowledge, Docker has never been applied before for entomological purposes, and it makes this short communication pioneering such as Rossini et al. (2019a), where the use of ROOT outside its native field of application was discussed for the first time.

The second major change concerned the graphical representation of the simulations, which has been entrusted to a Python script for a faster visualization through the "*dash*" and "*plotly*" packages. With this change, necessary for *EntoSim* to work into Docker without any X-server support, the results will be visualised in a smarter way directly on the internet browser, simplifying the use of the software on remote machines, also. The third major change was the addition of two more population density models (Rossini et al., 2020a, 2020c).

Lastly, a complete dataset has been also provided within the *EntoSim* Docker image, so that the users could familiarize with the software and reproduce the same results and graphs, to later move to their own research projects.

2. Materials and method

Insects, and ectotherms in general, are strongly dependent by the external environment. Since the first experimentations towards this direction (Harcourt, 1969), temperature was considered the main driving variable for insects-development (Colinet et al., 2015). This led, along the years, several researchers to find mathematical expressions linking the average temperature of the living environment with the insects' development time (Damos and Savopoulou-Soultani, 2012; Ikemoto and Kiritani, 2019). Theoretically, each species has a "*thermal spectrum*" (Rossini et al., 2019b), namely a range of temperatures bounded by a lower and an upper threshold between which the development of the species is allowed (Shi et al., 2017). Inside this range there is an optimal temperature, which is, by definition, the value where the species closes its life cycle in the shortest time (Quinn, 2017). Hence, the development time is as longer as the environmental temperature is far from its optimal value and near to the thresholds (Mirhosseini et al., 2017).

This typical increasing/decreasing profile is well described by empirical and not empirical expressions, already involved into the initial version of *EntoSim*, as reported in Rossini et al. (2020c, 2019a). More specifically, the expressions included within *EntoSim* are the Briére (Briere et al., 1999), the Logan (Logan et al., 1976), the Sharpe and De Michele (Sharpe and De Michele, 1977), and the linear (Damos and Savopoulou-Soultani, 2012; Severini and Gilioli, 2002) development rate functions.

The major mathematical contribution to discuss in the current version of *EntoSim* is represented by the implementation of new population density models, whose mathematical details and validations were already discussed in the cited literature. The availability of multiple population density models and development rate functions in a single software allows a faster analysis and comparison: in this way the user has a wider scenario about the best combination of phenological and population density models for her/his specific use. The selection criteria of the most suitable development rate function and the most suitable population density model were discussed by Rossini et al. (2020a), and can be also extended to all the physiologically based models.

Besides the Manetsch's Distributed Delay Model (Manetsch, 1976; Vansickle, 1977a) and the Generalised Von Foerster's equation (Rossini et al., 2020d, 2020f, 2019b; Vansickle, 1977b; Von Foerster, 1959) two additional population density models were added in this version of *EntoSim*. The first one is a revised form of the Manetsch's Distributed Delay Model (Rossini et al., 2020a), which expresses, as solution, the distribution of the individuals within the life stages.

The insertion of this revised version of the Distributed Delay Model in *EntoSim* would be beneficial to the wide set of users which are still confident with the Distributed Delay Model theory. The classical version (Manetsch, 1976; Vansickle, 1977a), in fact, describes the flow of individuals exiting from each stage, while its revised version has, as solution, the number of individuals which are present in each life stage.

However, the difference of behavior of these two versions of the model has not been widely explored enough. *EntoSim* can promote the comparison between the two model versions and future validations in other case studies of entomological relevance.

One of the main concerns in applying physiologically based models in varying temperature environments is the absence of an expression which designates (exactly) the daily temperature variations (Rossini et al., 2020f). Accordingly, this value is usually provided by direct measurements with meteorological stations and inserted into the development rate functions, requiring numerical solutions to solve the population density models.

The second population density model introduced with this version of *EntoSim* is a generalised form of the Von Foerster's equation with a reproduction term (Rossini et al., 2020c).

The third block of *EntoSim*, instead, concerns the validation or, more in general, the comparison between two or more data series. In the initial version of the software only the χ^2 function was used as overlapping index (Rossini et al., 2020d). In this revised version, instead, χ^2 was supported by the coefficient of determination R^2, in order to make applicable the protocol analysis proposed by Shi et al. (2017), Rossini et al. (2020a) and Bellocchi et al. (2011).

On the side of the programming language, the choice of C/C++ and the ROOT's libraries was maintained: they still manage all the calculations and fitting operations, respectively, but in this revised version, Python language was chosen for the graphical part. The reasons behind this choice are manifold: firstly, the capability to visualise results directly on a web browser page results into a faster option if compared to ROOT's *TApplication*. This become a key factor when *EntoSim* has run in remote machines, since the visualization using an internet browser is faster than using the Linux or MacOs X server. Secondly, using Python instead of ROOT's *TApplication* gives to the end-users the possibility to reverse back directly to the *EntoSim* menu, instead of restarting the executable code each time.

As already stated in the Introduction, the most important novelty on the programming and deployment side is the use, for the first time in entomological contexts of 'containers' technology based on Docker runtime (Docker, 2021). In fact, as the complexity of *EntoSim* increased, the runtime dependencies become complex as well as risking to miss some library objects at build time.

A Docker image can be considered as an executable software package including the essential to run the specific program, from the source code to the system tools, libraries, and other settings. In simple words, a Docker image container is similar to a virtual machine but with the great advantage to be more efficient, since it virtualizes the operating system instead of the hardware. Hence, once a Docker container image is developed, the user needs only to install the Docker engine on its computer, which is available for all the operating systems and makes the runtime of the containers the same in every machine.

The *EntoSim* Docker image was built through a Dockerfile, "*a text document that contains all the commands a user could call on the command line to assemble an image*" (DD, 2020) and made it available on GitHub page of *EntoSim* (ESGHP, 2021).

Proceeding by order, the first dependence provided into the Dockerfile was a base version of Linux CentOS 7 (LC, 2020). Since this version has only the essentials packages, the following commands inserted into the Dockerfile concerned the update of the existing CentOS packages and the installation of the dependencies required by ROOT. Subsequently, the Dockerfile provided for the installation of Python v3.6 and its packages *plotly*, *pandas*, *dash* and *numpy*.

At this point, the environment of the Docker image was suitable for the *EntoSim* installation that, to simplify the operation, has been entrusted to the related Makefile. The Makefile compiles the source code and builds three libraries containing the functions which supports the three blocks of the software, namely "*fittasso*", "*simulator*" and "*validator*".

The *EntoSim* Docker image is stored on the dedicated repository (ESDP, 2021) and it is available to the users through the Docker pull service (DD, 2020). In this way users have just to pull the image from the Docker repository to use *EntoSim*; moreover, it is possible to remove and pull it again every time there is the need to make the space available on the hard drives or when an update is made available by the developers. It is worth to mention that the Docker image solves all the problems of installation and compatibility, but the *EntoSim* code has been made available on GitHub for the users who wants to: *i)* compile and install it from the source code (solving all the dependencies by themselves) and *ii)* contribute to *EntoSim* with novel functionalities.

A schematic representation of *EntoSim* within the Docker image is shown in Fig. 1. *EntoSim* is composed by a main menu, printed on the computer shell, which recall the three main "macro-steps" of model application: *fittasso*, *simulator* and *validator*.

In the next section, a brief application of the software has been reported as result, considering literature data about the case study of *Tuta absoluta* (Meyrick) from Özgökçe et al. (2016). This case study is contained into the Docker image as working example for the users.

3. Results

Once the user has downloaded and run the *EntoSim* Docker image, following the instructions provided, she/he is ready to use the software for its own purposes. To allow the transfer of input/output files, a dedicated folder, *EntoSim-data*, has been created into the Docker container so the user may mount its data directory (typically the user's local homedir) at container start time. Hence, through this folder, the user can insert the input files in the specific *EntoSim*'s input folders and store the results in the local machine copying them from the *EntoSim*'s output folders. The first block of *EntoSim* is "*Fittasso*" composed, in turn, by six functions. The first function converts the experimental life tables data series from temperature-mean development time format in temperature-development rate format. As shown in Fig. 1, four *Fittasso* functions manage the non-linear fitting operations with the development rate functions, providing the results both in a graphical form on a web browser page and stored into specific ASCII text output files.

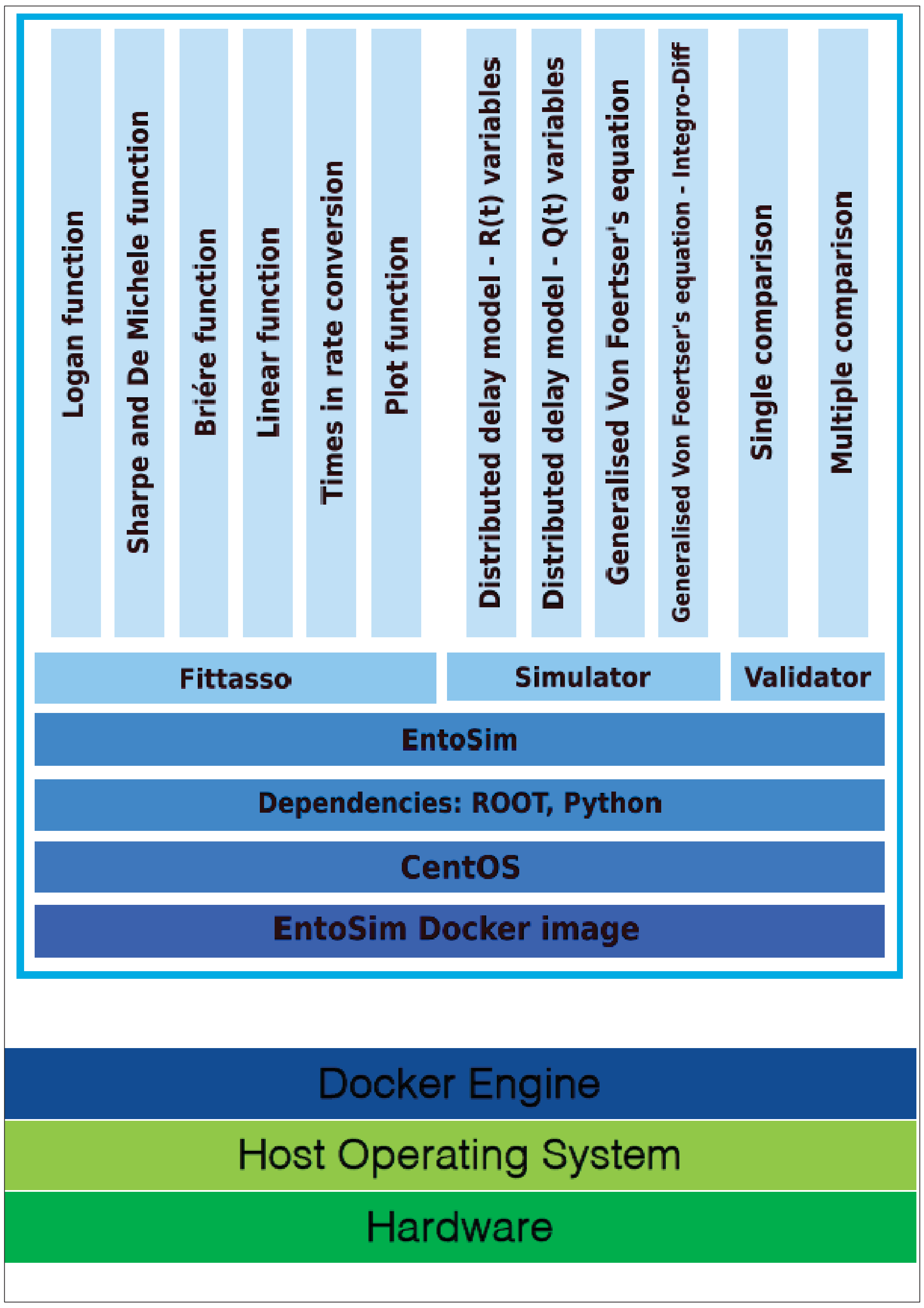

Fig. 1. Schematic representation of *EntoSim* docker image and how it is related to the computer hardware and operating system

For a visual inspection, fit results are displayed on the computer shell: in such way the user can quickly see if the results are satisfying or not. The best fit parameters of the development rate function are stored, also, in a hidden folder, so that "*Simulator*" can directly take these values as input. The last function involved in *Fittasso* allows the user to show the resulting best fit functions, provided by the previous operations, overlapped in an interactive single plot with life tables data.

A working example of this first block of the *EntoSim* is provided in (Fig. 2) in the case of *T. absoluta*. Once the life tables data from Özgökçe et al. (2016) are inserted, and once the parameters of all the development rate functions are estimated, a graphical resume is important to select which is the most representing function for the dataset and for the species under study. Even though the χ^2 and R^2 values are a valuable indication of the best fit function, it is worth to keep in mind that the final choice is weighted also by the biological meaning of the functions' parameters and by the experience of the users in respect of the species simulated.

The second block of *EntoSim* is "*Simulator*" (Fig. 1) composed, in turn, by four functions: each for each population dynamics model involved, that is the Manetsch's DDM, its revised form, the generalised Von Foerster's equation and the generalised Von Foerster's integro-differential equation. Once the user selects a model, the input files are automatically absorbed from specific folders. More specifically, the number of inputs changes with the model selected, while the outputs are provided all in the same way. The latter are stored in specific .txt files, to be utilised in further analyses, and plotted in a web browser page in three tabs. The first tab hosts a 3D representation of the population density with stage and time as independent variables (Fig. 3); the second tab hosts a plot where the population densities over time provided by simulations are overlapped (Fig. 4) and the third tab hosts multiple plots, each of those reports the population density, over time, of the simulated life stages.

The working example provided in Fig. 3 and Fig. 4 is referred to simulations in the case of *T. absoluta* using the generalized Von Foerster's equation as population dynamics model, and the Sharpe and De Michele development rate function as input. Temperature data, instead, are not referred to a particular case study, and were generated randomly (considering an optimum for the species of 32 °C) only for demonstration purposes.

The third and last block of *EntoSim* is "*Validator*". This tool was initially thought to estimate the *h* value needed by the Manetsch's DDM (Rossini et al., 2019a), but in the course of time its usefulness has grown. It is composed by two functions (Fig. 1) with similar tasks. Proceeding by order, the first function of *Validator* calculates the χ^2 and R^2 values comparing only two series of data; results are then provided both in numerical (a .txt file) and graphical form (a QQ-plot). The second function of *Validator*, instead, allows users to compare a data series (which may be validation data or theoretical values) with all the simulations provided by *Simulator*. Then the results are stored in a .txt file and ordered from the highest to the lowest overlapped on the basis of the χ^2-value. The aim of *Validator* is to provide the user a tool to quantify the overlap between data series and beyond. In fact, it is possible to compare: *(i* validation data with simulations; *(ii* different outputs provided by different models, or *(iii* outputs by the same model with different development rate functions in input, supporting the *a priori* and *a posteriori* analysis introduced by Rossini et al. (2020a). The *EntoSim* code was organised in separated modules, so that just minimal modifications of the existing code are typically required to implement new features.

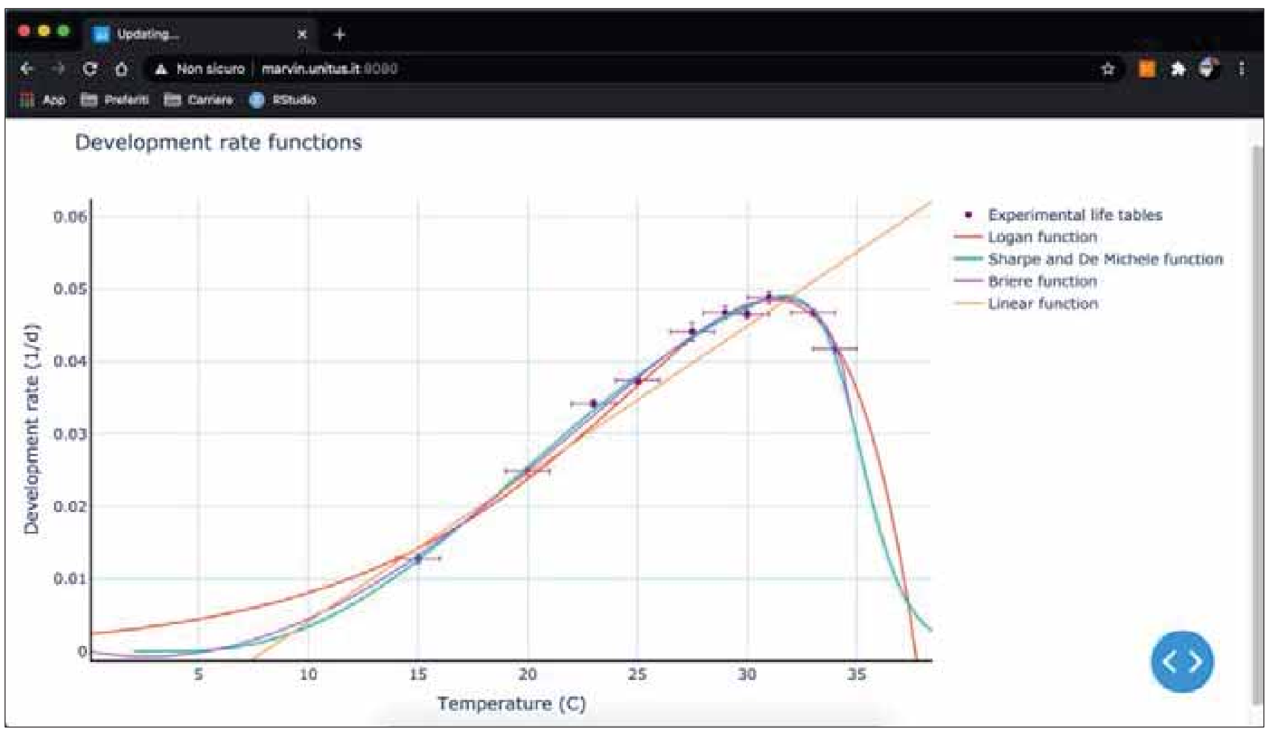

Fig. 2. Visual result of *Fittasso*. This output provides an overlap of the best fit functions, calculated by *Fittasso*, and of the experimental life tables. Plot are shown in the internet browser in an interactive mode, so that the user can zoom specific part of the plot or visualize/remove plotted functions. As example, the life tables of the tomato leaf miner *Tuta absoluta* (Meyrick) from Özgökçe et al. (2016) were used, as showed by Rossini et al. (2019b).

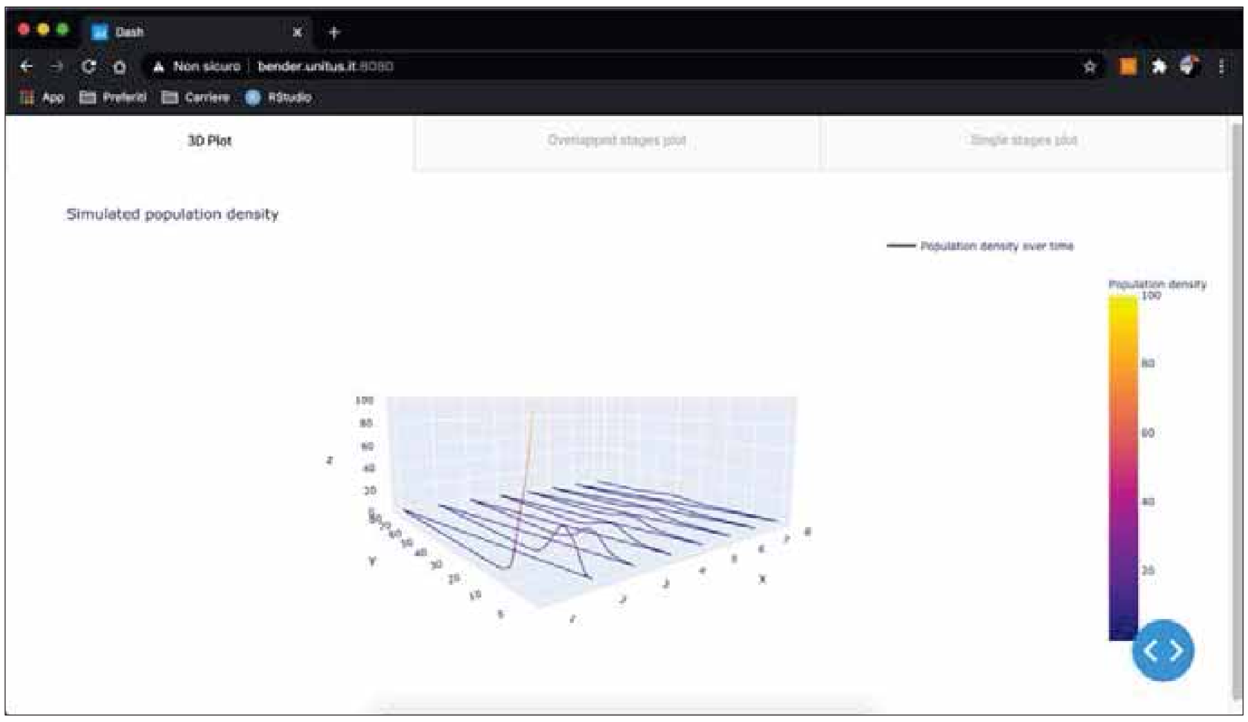

Fig. 3. Visual result of *Simulator*. A triad of plots is shown in an internet browser webpage.
In this specific picture a 3D plot of the simulated population density developing over time and through the life stages is reported

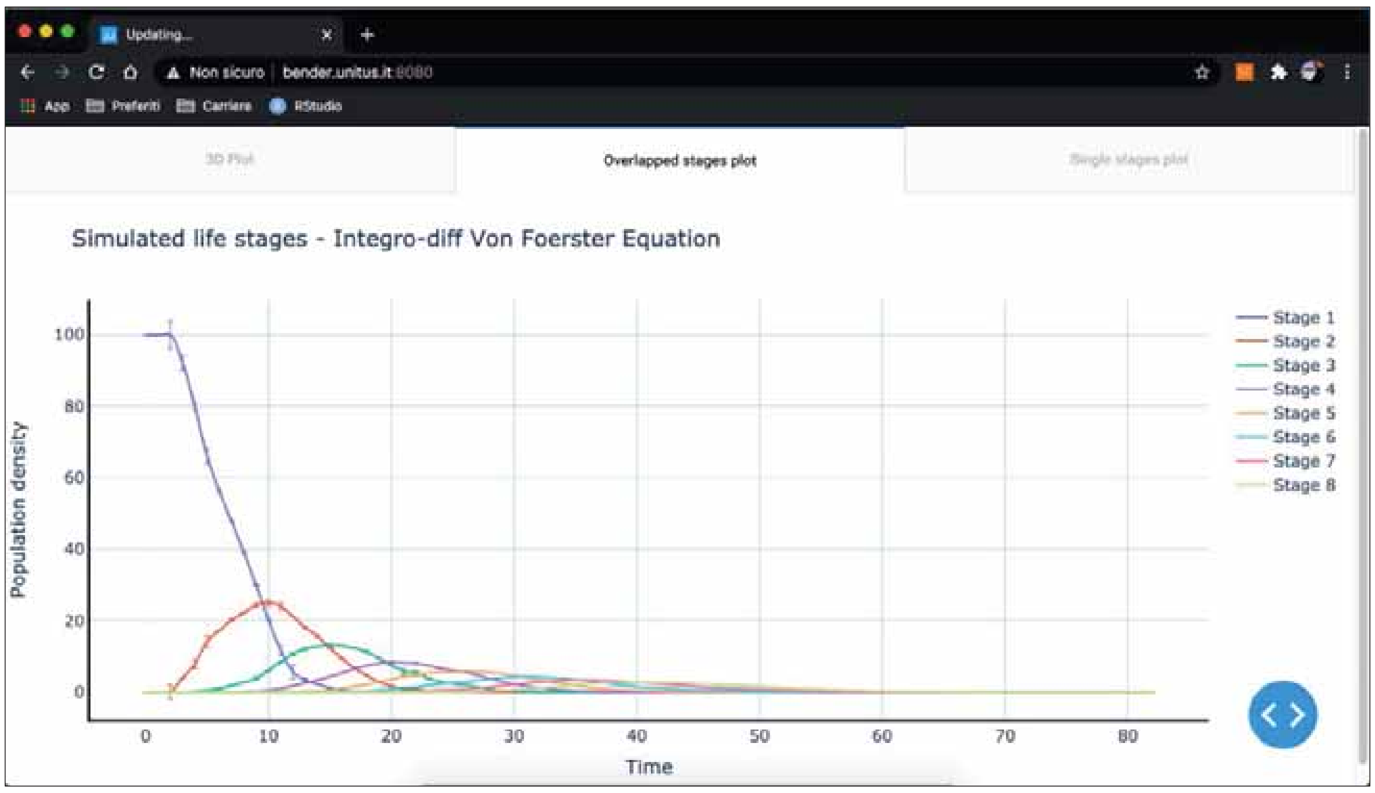

Fig. 4. Visual result of *Simulator*. A triad of plots is shown in an internet browser webpage.
In this specific picture an overlap of the simulated life stages over time is reported

This can foster future software developments: for instance, if a new function is required by the user, it is possible to develop only the dedicated module. Subsequently, the latter can be inserted into *EntoSim* only modifying the menu and the code of the block of destination.

4. Conclusions

Since its first introduction, *EntoSim* aimed to support a faster application of physiologically based models for decision making in agriculture, forest and ecological sciences. The inclusion of *EntoSim* into a Docker image introduced with the present work endorse the *EntoSim* shareability and development, providing a powerful tool to the insiders.

The development and validation of new models describing the same natural phenomenon, in fact, increases the need of an easier model application and comparison of their outputs. The use of Docker complies with this aim, and with a better reproducibility of the results in entomological modelling.

Thus, a modular software enabling multiple physiologically based models, as well as *EntoSim*, is a great resource for scientists, technicians, and farmers, since they could find the better combination of phenological and population density models for their specific use. Furthermore, an open-source code software, with a high shareability, strongly reduces the costs of development and distribution, in favour of the users with limited economic resources. This is the main reason of why the *EntoSim* code was made available on two different repositories: the Docker image makes the use of *EntoSim* easier, but at the same time the GitHub source code allows future development and contribution from the scientific community.

In the future the purpose is to enrich even more *EntoSim* with new functions, as well as to simplify the operations. In this regard, the development of a web application to substitute for the actual menu would be beneficial to the less specialised users.

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