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DOI
10.1016/B978-0-443-15274-0.50365-6

Publication date
2023

Document Version
Final published version

Published in
Computer Aided Chemical Engineering

Antonis Kokossis, Michael C. Georgiadis, Efstratios N. Pistikopoulos (Eds.)
PROCEEDINGS OF THE 33rd European Symposium on Computer Aided Process Engineering (ESCAPE33), June 18-21, 2023, Athens, Greece
 http://dx.doi.org/10.1016/B978-0-443-15274-0.50365-6

Paving the way for the integration of synthesis, assessment, and design tools within an ontological framework

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Abstract

The constant development of new alternatives to treat waste aids in closing material loops towards the circular economy and improving sustainability through the use of new renewable materials and energy. This fact leads to the increasing need for decision-making tools for process synthesis and assessment, which can be addressed with an integrated framework that employs ontologies for knowledge management and optimization tools to perform a hierarchical assessment of alternatives. The systematization of these procedures raises the need for tools to automate techno-economic and life cycle analyses. In this work, such a challenge is addressed through the additional integration of add-on modules such as the CapEx-Opex estimation tools and surrogate modeling within this framework. A case study on plastic waste is proposed with the inclusion of several pyrolysis and gasification alternatives. Results show pyrolysis, followed by the subsequent purification of its products, as the best alternative and helped identify main drivers for technologies feasibility such as feedstock purity and energy consumption.

Keywords: circular economy, integrated modeling, sustainable development, machine learning, economic optimization.

1. Introduction

The Circular Economy appears as a subject of paramount importance toward economically, environmentally, and socially sustainable development. Thus, many entities across the world are working hard to find alternatives that not only bring economic profit but also are environmentally benign and socially responsible. One of the most urgent matters is waste management and, in this specific line, many technical efforts are currently devoted to finding new waste-to-resource processes, recovering valuable resources, and closing material loops. Consequently, decision-makers face the challenge to determine which alternatives are most suitable for each kind of waste. To address this task, Pacheco-López et al., (2022) developed a framework of integrated tools to connect waste sources with valuable products and find the best routes to close material loops. The application of this framework requires performing economic and environmental analyses and developing models suitable for each one of the alternatives included. To undertake these tasks more systematically, this contribution aims to integrate new tools to make the framework more versatile and minimize the required human intervention for synthesizing and assessing new sustainable approaches. Within the proposed framework, the ontology is used to manage the information and data that are needed as inputs on each module, as well as storing the outputs, therefore centralizing all the knowledge required and produced in the system (orange arrows represent information exchange in Figure 1).

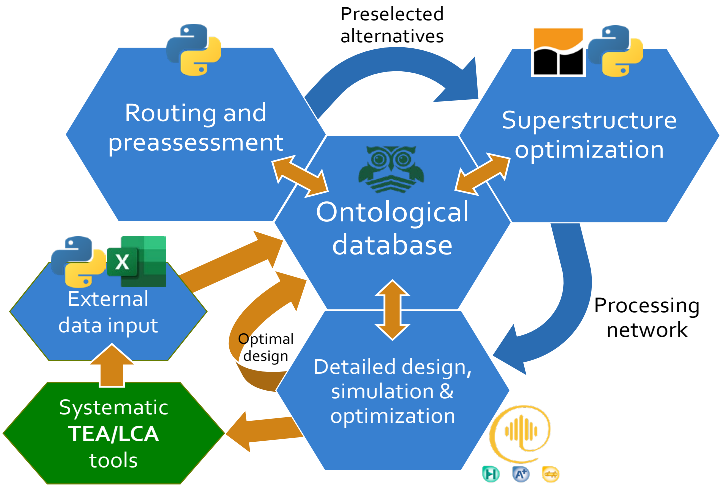

Figure 1. Schematic representation of the proposed framework with an additional module (green).

2. Methodology

The methodology used in this contribution is an extended version of a previously proposed one, in which several synthesis, assessment, and optimization tools were integrated to build a decision-making framework (Pacheco-López et al., 2022). There, a sequential approach is used to build alternative paths between waste materials and marketable products and to assess them from several points of view as well as to find the optimal configuration. First stage uses a new proposed algorithm and metric based on different objectives to pre-select alternatives, then a second stage consisting on a Multi-objetive network optimization to find best routes based on each objective (for more details of this procedure see (Somoza-Tornos et al., 2021)). One of the identified challenges in this work was the need to perform previous techno-economic (TEA) and life cycle (LCA) assessments manually for every single process in order to introduce their results in the framework to be used by the other modules. To address this challenge, the need for systematization tools was identified to reduce human intervention and standardize the results. In this direction, some tools were already developed and are being implemented in the framework. Prifti et al. (2022) developed a CapEx-OpEx Robust Optimizer (CORO) framework that was intended to assess the cost evaluation of a plant including some sustainability targets, thus, it provides the framework with more dynamism and systematization in the TEA tasks. CORO automatically takes a simulation file (Hysys or ProII) as an input and generates the capital and operational expenditures for each process. Using this tool, the cost estimations for all processes in the ontology have been performed in order to obtain standardized results. Figure 1 shows the original methodology and the proposed additional module for techno-economic/life-cycle systematic assessment tools.

As of now, only systematic TEA is implemented for illustrative purposes, although future developments are intended to include LCA systematization in the same way.
On the other hand, process simulation is also a critical step for the design and optimization of new processes, which, in turn, may require considerable computational effort. Surrogate modeling offers the possibility to speed up simulation convergence times by substituting rigorous models with machine learning methods (Granacher et al., 2021), as the one proposed by Galeazzi et al., (2022) to predict the behavior of several process variables of existing steady-state digital twins of industrial plants. This tool can be accessorily used in the third stage of the methodology to ease the simulation step or to study the processes' sensitivity to variations in feed composition or operating conditions.

Table 1. Deployed process paths for MPW treatment, outputs, and GPI for 24 alternatives. Sor.: Sorting; FBR: Fluidized bed reactor; HGHTR: horizontal gas heated tube reactor; ZSM5: ZSM-5 zeolite; FCC: fluid catalytic cracking; R1: FCC-R1 commercial FCC equilibrium catalysts; HUSY: Ultrastabilized Y zeolite; SAHA: amorphous silica-alumina; HZSM: acid zeolite; SA9Z1: hybrid catalyst (SA: Zeolite, 9:1); LPG: C1-C3 aliphatics.

	Processes	Outputs	GPI
1-3	Pyrolysis 500ºC R1/Red Mud/ZSM5/	C1-C5 alkanes, ethylene, H2, hexene, toluene, ethylbenzene, styrene, naphthalene, xylene & C9-C14	723-642
4	Pyrolysis 600ºC /Y zeolite/	Methane, ethylene, propene, ethane, butane, butane, hydrogen, benzene, toluene, ethylbenzene & styrene	558
5-8	Acid FCC 390ºC /HUSY//SAHA/R1/ZSM5/	Gasoline, LPG, light aromatics mixture, C9-C14 mixture, char & HCl	435-425
9	Gasiforming	Methanol & CO_2 credits	288
10	Sor. + PE pyrolysis 520ºC HGHTR /ZSM5/	Gasoline, ethane, propane, butane & char	216
11	Sor. + PE pyrolysis 740ºC	LPG, ethylene, benzene, toluene, indane & pyrene	183
12-13	Sor. + PE pyrolysis FBR 375ºC /HZSM/SA9Z1/	Gasoline, ethane, propane, butane & char	151-116
14	Sor. + PP pyrolysis 350ºC	WPPO (diesel substitute) & char	96
15	Sor. + PE pyrolysis 1000ºC	Methane, ethylene, propene, butadiene & benzene	87
16	Sor. + PP pyrolysis 760ºC	LPG, ethylene, benzene, toluene & naphthalene	79
17	Idem + Ethylene hydration	LPG, ethanol, benzene, toluene & naphthalene	70
18	Co-gasification 850ºC	Methane, ethane, syngas & char	63
19	Gasification 850ºC	Methane, ethane, syngas & char	59
20	Electrified Gasiforming	Methanol & CO_2 credits	54
21	Sor. + PS pyrolysis 425ºC	Toluene, styrene, cumene & 1,3,5-triphenylbenzene	42
22	Sor. + PE pyrolysis 550ºC	WPPO (waste plastic pyrolysis oil – diesel substitute)	35
23	Incineration	Energy Recovery	0
24	Landfill	None	0

3. Case Study

The framework is tested on a case study dealing with the recovery of plastic waste materials and the conversion/purification of the resulting products into other valuable carbon-based products. New alternatives are added to the set of alternatives available in the ontology from previous implementations using the same assumptions as presented in Pacheco-López et al., (2022). These new processes consist of gasification followed by methane reforming and conversion to obtain methanol as a final product, either using

traditional energy sources or electrified ones (Prifti et al., 2021). A total of 66 processes (see Figure 2) are implemented in this case, where 200 paths were created and assessed, from which 24 were selected in the first stage (see Table 1).
The preselected alternatives were sent to the multi-objective network optimization module obtaining a set of configurations along with the representation with the corresponding Pareto fronts. The newly added alternatives are compared against those already available in the ontology. The feedstock considered corresponds with a mixture of plastic waste with the following mass composition: 45% polyethylene, 32% polypropylene, 20% polystyrene, and 3% of PVC. A plant to treat an annual amount of 20,000 tonnes of MPW (2.5 tonnes/hour for a plant operating 8000h a year) was considered and all processes were scaled accordingly.

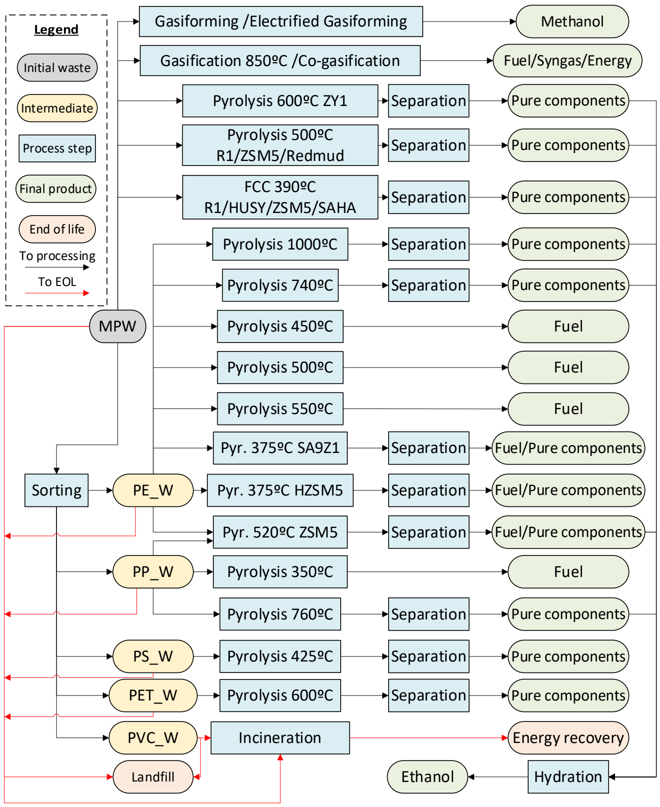

Figure 2. Implicitly generated graph in the pre-assessment stage with all tentative connections. PE: polyethylene, PP: polypropylene, PS: polystyrene, PET: polyethylene terephthalate, PVC: polyvinyl chloride; Pyr.: Pyrolysis; EOL: End of life.

4. Results

After updating the ontology with all the current and new process parameters, the algorithm is run and all the possible connections are made with an input-output matching procedure, resulting in a graph as seen in Figure 2. With the assessment procedure presented in Pacheco-López et al., (2021), all the paths are built and a list of prioritized alternatives is obtained and preselected according to their global performance indicator (see Table 1, for brevity similar routes have been combined). This prioritized list of alternatives is passed to the network optimization stage where a multi-objective optimization is performed. A set of different process configurations is obtained according to different objectives and intermediate alternatives as well as a set of Pareto points using the ε-constraint method. As an example, the configuration with the best economic performance is shown in Figure 3 along with the Pareto fronts obtained for the economic profit against each one of the environmental endpoint indicators as shown in Figure 4.

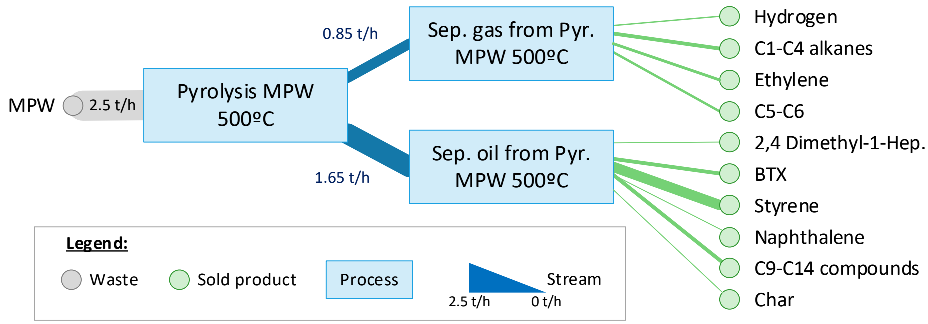

Figure 3. Configuration obtained for maximized profit. Point number 10 in Figure 4.

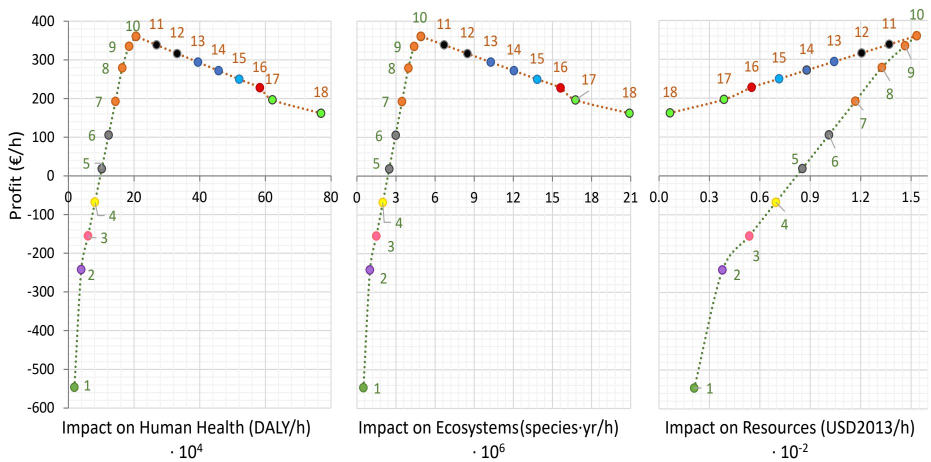

Figure 4. Pareto fronts for the trade-off between profit and the three environmental endpoint indicators. The points are numbered and color-coded to represent different configurations. Each point (as the one seen in Figure 3) consists of a different combination of processes from Figure 2.

Results in this contribution were consistent with those obtained in previous runs of the algorithm (Pacheco-López et al., 2022, 2021). Newly introduced gasification alternatives were selected in the first stage in the positions 9th, for the traditionally powered route, or Gasiforming^{TM}, and 20th, for the Electrified Gasiforming^{TM}. In addition, they were not among the best-performing alternatives in the second stage for any of the four obtained anchor points, which may suggest they need further development and more efficient and economically competitive energy sources. It was identified that capital expenditures play an important role in the implementation of these technologies. Electrical energy consumption has been also identified as a critical part since it entails most of the operating expenditures. On the other hand, results show that pyrolysis of mixed plastic waste with or without catalysts at a temperature of 500ºC is still among the best-performing alternatives for most objectives since they are the most economically and environmentally competitive or beneficial options for this kind of waste.

5. Conclusions

Results show the framework's ability to synthesize and assess routes for the upcycling of waste accounting for economic and environmental objectives. The capability of the framework to be easily expanded and complemented with the integration of other tools to satisfy processes modeling, design, and assessment needs has also been proven. The use of the CapEx-OpEx Robust Optimizer (CORO) has aided in systematically generating the economic performance indicators for all the processes asserted in the ontology, providing a standardized procedure to avoid user-introduced errors and keeping the assessment parameters consistent among all alternatives. The third stage of the methodology, detailed simulation, and design of a chosen alternative is one of the most work-intensive tasks of the framework and stays out of the scope of this study. The use of surrogate modeling has been envisaged as a useful alternative to ease this stage and might be implemented in future developments to study the effect of feedstock composition changes on the economic and environmental performance of the upcycling technologies. Some identified challenges have been approached with the inclusion of new ideas and tools that help advance the automation and systematization of the framework, mainly in terms of TEA/LCA and simulation efforts. The possible inclusion of carbon emission credits has also been included as a potential source of income, therefore improving the overall economic performance of the considered alternatives.

6. Acknowledgments

Financial support received from the Spanish "Ministerio de Economía, Industria y Competitividad" and the European Regional Development Fund, both funding the research Project CEPI (PID2020-116051RB-I00) is fully acknowledged. A.P-L thanks the financial support received from the "Ministerio de Ciencia e Innovación" (grant ref. PRE2018-087135) and the Erasmus+ programme of the EU 2021-27 (KA131 call).

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