

# Pyrolysis of plastic waste: UniSim Design© simulation case study for renewable energy production

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## Highlights

- Experimental results from lab-scale pyrolysis aim at increasing gaseous fuel production.
- Unisim Design© allows to perform an effective thermal process integration.
- The GHG emissions from simulation software will be the basis for emission savings assessment.

## 1. Introduction

Fossil fuels, despite their environmental impact on Earth, remain the primary energy source globally. Many countries are transitioning to renewable energy, aiming to enhance energy efficiency and combat climate change, as outlined in their nationally determined contributions under the Paris Agreement [1]. However, achieving the set targets for global renewable energy capacity requires substantial investment, hindering progress. Recycling plastic solid waste (PSW) for chemical and fuel production is considered as a valuable alternative, given the high volatile content in PSW that can yield fuels and energy. Thermochemical conversion, particularly pyrolysis, is a promising technology for transforming plastic waste into renewable energy sources with lower environmental impact [2,3]. The European Union's Recast Renewable Energy Directive defines recycled carbon fuels (RCFs) and establishes criteria for considering them renewable, focusing on a minimum 70% reduction in greenhouse gas emissions compared to fossil fuels. Therefore, the main goal of this work is to assess environmental impacts coming from pyrolysis of plastic scrap, derived from the densified polyolefin production process; to this aim, a selected industrial scenario will be implanted using a dedicated software (i.e., Unisim Design©) and thermal integration, combined with the usage of gaseous co-product for sustainable energy production, will be carried out. The simulation outcomes will be used, in a future work, to evaluate the emissions savings according to the Directive.

## 2. Methods

PSW underwent to a double-stage thermal pyrolysis. Experimental results guided the modeling simulation for predicting PSW pyrolysis plant performance, enabling process optimization for industrial-scale efficiency. UniSim Design© was employed to create a flowsheet, evaluating operative conditions, material, energy balances, and utility requirements. Using the Peng–Robinson thermodynamic property fluid package, hydrocarbon and light gas components are accurately modeled. Through DSC analysis, polyethylene (PE) was identified as the main hydrocarbon in PSW and modeled using UNIFAC group contribution methods. The pyrolysis process was modeled, considering gaseous compounds ( $H_2$ ,  $CO$ ,  $CO_2$ ) and hydrocarbons ( $CH_4$ ,  $C_2H_4$ ,  $C_2H_6$ ,  $C_3H_6$ ,  $C_4H_8$ ) for energy balance computation. Yield shift reactors simulated both pyrolysis units, calculating thermal energy requirements for maintaining constant temperatures. The resulting vapor-liquid stream was separated in *E-1* and *V-1* to isolate octane and octacosane. The internal combustion engine (ICE) simulation involved combustion of pyrolytic gases, cooling, and thermal power recovery. Process simulation, with a PSW mass flow rate of 200 kg/hr, explored two energy supply scenarios for pyrolysis reactions: fossil fuel combustion (scenario A) and thermal integration of process streams (scenario B). In scenario B, recovered thermal duty was used for heat integration in the first stage and for pre-heating air used for pyrolytic oil combustion reaction. The heat integration excluded the second stage reactor, assuming autothermal behavior due to partial combustion of pyrolytic vapors.

