DOI: https://doi.org/10.15446/ing.investig.119991

Research Article/ Mechanical, Mechatronics, and Materials Engineering

Systemic Analysis and Synthesis for Modeling the Pyrolysis of Plastics: Estimating the Optimal Operating Temperature

Análisis sistémico para el modelado de la pirólisis de plásticos: estimación de la temperatura óptima de operación

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ABSTRACT

In the reviewed literature, experimental and simulation methods prevail as the main tools for developing technologies for converting plastic waste into synthetic fuels. This paper proposes a methodology for determining the operating parameters for this conversion using high-density polyethylene (HDPE) as an example. To address the problem, a methodological approach based on engineering systems analysis and synthesis was used. This resulted in a conceptual mathematical model for developing HDPE pyrolysis technology, both general for process operation and specific for a basic facility design. A virtual experimental plan was executed using the Aspen Plus process simulation tool under thermodynamic equilibrium conditions. Based on the generated data, approximation functions for the efficiency indicators and the constrained functions required for parameterization were developed. Decisions were then made to determine the optimal pyrolysis temperature by iteratively optimizing the resulting detailed nonlinear multi-objective model, varying the desired values of the efficiency indicators. This procedure allows for the identification of a pyrolysis temperature that satisfies the preferences of potential decision-makers and establishes the conditions for addressing the general problem posed for the operation of the conversion process.

Keywords: pyrolysis of plastics wastes, transformation of plastics into fuel, process operation modeling, methodologies for the analysis and synthesis of engineering systems

RESUMEN

En la literatura revisada, los métodos experimentales y de simulación predominan como las principales herramientas para el desarrollo de tecnologías de conversión de residuos plásticos en combustibles sintéticos. El objetivo de esta investigación fue desarrollar una metodología para determinar los parámetros operativos para esta conversión, utilizando polietileno de alta densidad (HDPE) como ejemplo. Para abordar el problema, se empleó un enfoque metodológico basado en el análisis y la síntesis de sistemas de ingeniería, el cual dio lugar a un modelo matemático conceptual para el desarrollo de la tecnología de pirólisis de HDPE, tanto general para la operación del proceso como específico para el diseño básico de una instalación. Se ejecutó un plan experimental virtual utilizando la herramienta de simulación de procesos Aspen Plus bajo condiciones de equilibrio termodinámico. Con base en los datos generados, se desarrollaron funciones de aproximación para los indicadores de eficiencia y las funciones restringidas requeridas para la parametrización. Posteriormente, se tomaron decisiones para determinar la temperatura óptima de pirólisis mediante la optimización iterativa del modelo multiobjetivo no lineal detallado resultante, variando los valores deseados de los indicadores de eficiencia. Este procedimiento permite determinar la temperatura de pirólisis que satisface las preferencias de los potenciales tomadores de decisiones y crea las condiciones para resolver el problema general planteado para la operación del proceso de conversión.

Palabras clave: pirólisis de desechos plásticos, transformación de plásticos en combustible, modelado de la operación de procesos, metodologías del análisis, síntesis de sistemas de ingeniería

Received: April 24, 2025
Accepted: December 16, 2025

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Introduction

Plastics are synthetic polymers characterized by their versatility, malleability, ease of processing, low density, favorable mechanical properties, thermal stability, chemical resistance, and moisture resistance, among other attributes [1, 3]. These properties, combined with their relatively low cost, have driven their widespread adoption across various industries, resulting in exponential growth in production over several decades [4, 5]. At present, the annual production of plastic is estimated at 430 million tons, out of which about 65% correspond to 'short-life' products that are rapidly discarded. Given their physicochemical properties, the natural decomposition of plastics can take hundreds of years. Consequently, plastic waste accumulates in ecosystems and can cause serious environmental damage, posing risks to flora, fauna, and human health [6]. Based on their structure, plastics can be classified as thermoplastics, thermosets, and elastomers, with thermoplastics accounting for about 80% of total production and being primarily used in the packaging and packing industries. These include high-density polyethylene (HDPE) [7], polyethylene terephthalate (PET) [8], polyvinyl chloride (PVC) [9], low-density polyethylene (LDPE) [10], polypropylene (PP) [5], and polystyrene (PS) [6, 11].

Plastic waste management commonly relies on recycling, sorting, and grinding for reuse. These strategies have been reported to achieve recovery rates between 15 and 20% [12]. Alternatively, thermochemical transformation technologies (pyrolysis, gasification, or combustion) can help reduce the volume of plastic waste by up to 90%, while simultaneously enabling the recovery energy and/or other by-products [13,14]. In the literature, abundant studies demonstrate the technical feasibility of the thermochemical transformation of plastics [15, 21], highlighting pyrolysis processes as viable technologies for obtaining biofuels or for stimulating gasification when the objective is synthesis gas. A critical analysis of the literature indicates that the nature or type of plastic, its size, the type of thermochemical transformation (pyrolysis or gasification), the configuration of the specific equipment where the transformation takes place (for example, continuous or batch equipment), the capacity of the installation (small, medium, or large scale), the operating conditions (such as flows, temperature and pressure), and even the heating systems and speeds, among many other variables, have a direct impact not only on the yields towards specific products (gaseous, liquid, or solid) but also on their quality [15, 21]. For instance, because plastic wastes such as LDPE, HDPE, PP, and PS are characterized by a favorable hydrogen/carbon ratio, energy efficiency, and higher calorific value, they are considered more promising as raw materials for pyrolysis, noted for their relative efficiency. Other materials such as PET, which contains considerable amounts of O_2 in its structure, may be more suitable in a gasification process. PVC should be handled with caution for use as a feedstock in a thermochemical transformation process, as the presence of Cl in its structure and the operating conditions can give rise to undesirable and sometimes dangerous contaminating by-products [22]. With respect to the operational decision-making problem associated with plastic-to-fuel transformation processes, the consulted literature predominantly reports solutions based on experimental studies and the application of simulation procedures. In this study, it is assumed that process operation problems in general, and the transformation of plastics into synthetic fuels in particular, should be subjected to the analysis and synthesis of engineering systems, mathematical modeling, and synthesis of the corresponding systems. Accordingly, this problem is formulated as a preparation and decision-making task, whose solution involves conceptual modeling, virtual simulation, descriptive modeling and systematic decision analysis, in accordance with the methodology described in [23] and [24]. This this paper is therefore based on the hypothesis that the solution to the operational decision-making tasks associated with the transformation of plastic into synthetic fuel should precede the physical experiments.

Due to the complex nature of the thermochemical transformation process and the number of variables that can affect its performance, experimental studies are usually conditioned by the availability of laboratory scale equipment. Consequently, studies involving pilot and/or industrial plants for data acquisition remain limited. For this reason, most of the reported contributions support their conclusions through the rational use of process modeling and simulation tools, such as Aspen plus, HYSYS, DWSIM, and CHEMCAD, among others. All of them are based on equations and mathematical models that represent the physical and chemical processes that allow (at different levels of detail) researchers to predict how the process is affected by changes in, or manipulation of, the input conditions, operating conditions, or even in design variables of the simulated equipment [14, 18].

Considering the growing accumulation of plastic waste and the need for robust mathematical modeling and simulation strategies to support the study, understanding, analysis, and eventual implementation of thermochemical conversion facilities, this article proposes a mathematical model that adequately describes process operation in general and, in particular, determines the optimal operating temperature of an installation, where the thermal decomposition of HDPE plastics is carried out. The selection of pyrolysis as the transformation technology and HDPE as the feedstock was intended to simplify the model. The model is presented innovatively, step by step, following methodologies proposed in the literature for systems analysis and synthesis in engineering [23, 24]. More specifically, a general model of the preparation and decision-making processes is constructed, and the relationship between the structure of this mathematical model and the decomposition structure of the corresponding task is examined. This task relates, as a rule, to multiple levels and criteria in which optimization, simulation, and graphical representation models are included.

As demonstrated in the following sections, the task to be solved has a multi-objective character, which determines the modeling approach to be used. Multi-objective optimization is strongly related to the articulation of preferences and when they are acted upon; never, before, during, or after the optimization process [25]. This has led to the development of different methodological approaches, including the absence of preference articulation (used when the decision-maker cannot articulate his preferences), *a priori* articulation of preferences (based on predefined objective priorities), *a posteriori* articulation of preferences (in which a Pareto front is generated and presented to the decision-maker), and progressive preference articulation (in which preferences are progressively adjusted to guide the search process).

For technological decision-making problems, the latter approach is the most suitable, as it allows decisions-makers to iteratively refine their preferences based on the observed behavior of the optimization results. The most commonly used methods in this category are the STEM [26] and Steuer's method [27]. The specialized literature presents other approaches that use the ideas of both methods, as is done, for example, in [24].

This methodology allows for the analysis of a wide variety of engineering problem classes (tasks) as multi-criteria preparation and decision-making tasks and associated optimization methods. The model developed under this framework is expected to be robust enough to serve as a basis for the study and optimization of similar systems adopting different configurations; in addition to representing a guide for the study and systemic analysis of the thermochemical transformation processes of plastics.

From an environmental perspective, this study is justified by the potential of pyrolysis to reduce the amount of plastics that end up in landfills or released into the environment, thereby contributing to a more sustainable waste management. The products generated (such as fuels and oils) can be used as raw materials for energy production or as input for new products, thus supporting circular economy principles and environmental sustainability. However, it is important to emphasize that reducing plastic production and consumption remains an essential component of any comprehensive strategy for addressing plastic waste. Additionally, the implementation of plastic waste pyrolysis processes can have positive social impacts; establishing pyrolysis plants can create direct and indirect employment opportunities in the construction, operation, and maintenance of the facilities, as well as in the collection and transportation of plastics. Furthermore, the promotion of recycling and resource recovery technologies, such as pyrolysis, can increase public awareness of waste management and sustainability practices in the community. Pyrolysis plants can contribute to local economic development by encouraging investment in infrastructure and services related to waste management. More broadly, the adoption of advanced waste management technologies can stimulate environmental research and development, promoting a culture of innovation.

The *Methodology* section provides a concise description of the adopted methodological approach, the descriptive models derived for the operation of the process deduced, the basic technological installation developed, the descriptive modeling procedures developed, and the description of the thermodynamic equilibrium model used in the virtual experiments.

The *Results and discussion* section subsequently detail the descriptive models, the optimization and decision-making procedures developed, and their application in obtaining solutions that adequately reflect the preferences of decision makers.

Methodology

Analysis and synthesis of engineering systems and their application to the development of plastic waste pyrolysis technology

Engineering decision-making tasks, regardless of their complexity, are subject to external and internal analysis and, on this basis, to the synthesis of the decision-making system (Fig. 1) [23, 24].

The modeling process begins with the systemic analysis methodology presented in [23] and [24], which comprises external and internal analyses. As a result of the external analysis, the set of variables associated with the decision-making task and a conceptual mathematical model are obtained. During the internal analysis, the mathematical description of the relations included in the conceptual model are found using accumulated domain knowledge and/or modeling techniques and tools available in literature. More complex tasks are decomposed, either by elements and/or by objectives, while simpler tasks can be solved directly. The analysis process may require several iterations. In the absence of established parameterization procedures, experiments may be required to identify the relationships that constitute the component models. These experiments may be physical or virtual in nature. The system synthesis involves the computational implementation of the detailed mathematical models resulting from the internal analysis, using existing tools or developing new ones for options generation, decision conciliation, simulation and/or complementary graphical representation. The following subsections present the step-by-step structuring of the model under this methodological approach, following the recommendations in [23, 24].

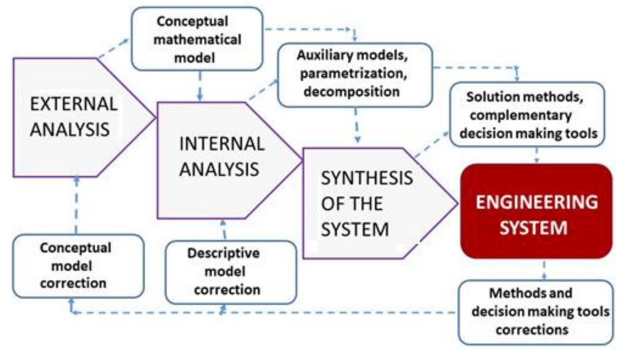

Figure 1. Illustration of the modeling process starting from systemic analysis
Source: Adapted from [23]

External analysis. The external analysis corresponds to the study of the largest task to which the system under analysis is subordinated. For this study, it corresponds to the general task of transforming plastic waste into synthetic fuel, independent of the type of plastic or the size (or type) of pyrolysis plant.

Coordinating variables. These are decision variables associated with the higher-level task that determine the link with the specific task under study. In this case, the following variables are defined: (i) type of installation (*TI*), *i.e.*, batch, fluidized bed, *etc.*; (ii) type of plastic (*TP*); (iii) basic dimensions (*Dalt*) that include the height (*h*) and width (*w*) of the workspace; (iv) the allowable lower pyrolysis temperature (Tzp^l); (v) the allowable upper pyrolysis temperature (Tzp^u); (vi) the required calorific power of the liquid fuel (PCL^l); and (vii) the required calorific power of the gaseous fuel (PCG^l). System pressure is not regarded as a significant variable, as plastic waste pyrolysis is mainly carried out at atmospheric pressure due to its lower operating costs compared to vacuum or high-pressure processes. In addition, it has been observed that fuel production during the thermal decomposition of plastic waste does not generally increase with pressure [25]. Therefore, its influence can be disregarded.

Efficiency indicators. Efficiency indicators characterize the quality of the potential solutions to the studied task and represent performance criteria of interest to the system user. Accordingly, the following indicators are proposed: (i) energy yield, *i.e.*, energy produced per unit mass of feedstock used (*RE*), (ii) liquid fuel yield, *i.e.*, volume of liquid fuel produced per unit mass of feedstock used (*RCL*), and (iii) installation cost (*Cost*).

Decision variables. These are the variables that can be manipulated by the system user to obtain the best possible compromise between efficiency indicators. The following decision variables are considered: (i) plastic flow rate (*CP*), (ii) granulometry (*GR*), and (iii) pyrolysis temperature (*T*).

Constrained functions. Constraint functions arise from physical limitations (of the equipment), natural (due to the substances used and/or phenomena involved), or imposed by the user (in terms of quality expectations, costs, etc.). For the analyzed system, the following constraints are defined: (i) pyrolysis temperature in the environment of possible values ($Tzp^l \leq T \leq Tzp^u$), (ii) calorific value of the liquid fuel ($PCL\ (TI, TP, DAlt, CP, GR, T, DFC, vc, tc, tr\ ) \geq PCL^l$), and (iii) calorific value of the gaseous fuel (PCG (*TI, TP, DAlt, CP, GR, T, DFC, vc, tc, tr*) ≥ PCG^l).

Conceptual model of the studied task. This model formalizes an approximation while considering the defined efficiency indicators. Following [24], this compromise is modeled as the minimization of the Tchebyshev distance from the desired values of these indicators to those calculated by the system. Within the proposed framework, the conceptual model is defined through the Multiple-Objective Function (1) and the Set of Expressions (2).

$$Max\ (RE, RCL, -Cost) \tag{1}$$

Subject to:

$$\begin{gathered} T \geq Tzp^l \\ T \leq Tzp^u \\ PCL(TI, TP, DAlt, CP, GR, T, DFC, vc, tc, tr) \geq PCL^l \\ PCG(TI, TP, DAlt, CP, GR, T, DFC, vc, tc, tr) \geq PCG^l \\ TI \in U_1 \\ TP \in U_2 \\ CP, T, DFC \in R^+ \\ GR \in x_2 \end{gathered} \tag{2}$$

where U_1 denotes the set of facility types considered, U_2 the set of plastic types considered, R^+ the set of positive real values, and X_2 the set of mesh sizes used after grinding.

Identifying the proposed model requires determining descriptive models for different types of installation, as well as prior knowledge of the liquid and gaseous products generated during pyrolysis in order to study the process kinetics. Therefore, preliminary approximations are necessary.

For the simplification of the model, a specific facility design and plastic waste is defined. High density polyethylene (HDPE) is chosen as the raw material because its molecular structure contains only carbon and hydrogen, which minimizes the generation of undesirable by-products during synthetic fuel production. In addition, HDPE is relatively abundant among single-use plastic waste. Regarding the facility design, a batch reactor configuration is adopted, considering dimensions and spatial requirements appropriate for operation in a research laboratory. The basic design of the plastic waste pyrolysis installation is illustrated in two views in Fig. 2.

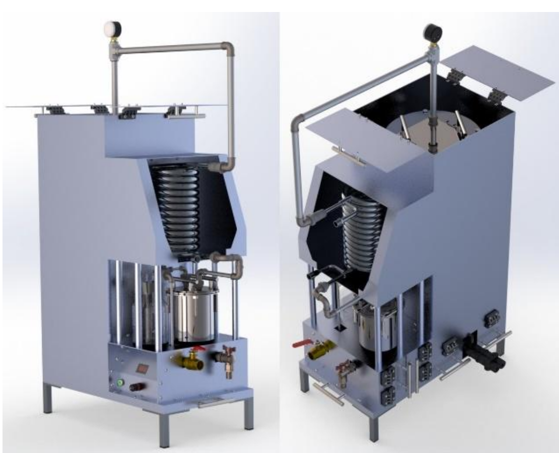

Figure 2. Illustration of a pyrolysis equipment for waste plastic pyrolysis
Source: Authors

The proposed reactor has an external diameter of 29.85 cm, a wall thickness of 6 mm, a total height of 67.63 cm, and an effective pyrolysis area of 60.14 cm. Heating is provided by a high-pressure gas burner which is placed under the reactor inside a rectangular insulation and protection structure. Condensation of the pyrolysis flue gases is illustrated in the form of a cylindrical helix as a water-cooling system. Non-condensable gases are collected in a storage vessel and are meant to be recirculated for use in reactor heating.

Under these assumptions, the model is simplified according to the Bi-Objective Function (3) and the Set of Expressions (4). By fixing the type of installation and the type of plastic, the only decision variable is the pyrolysis temperature, and the efficiency indicators are the energy yield (*RE*) and liquid fuel yield (*RCL*).

$$Max\ (RE, RCL) \tag{3}$$

Subject to:

$$\begin{aligned} T &\geq Tzp^l \\ T &\leq Tzp^u \\ PCL_{(T)} &\geq PCL^l \\ PCG_{(T)} &\geq PCG^l \end{aligned} \tag{4}$$

The Bi-Objective Function (3) can be reformulated using the Tchebyshev distance between the desired objective values and their existence space, *i.e.*, (3) can be replaced by (5) if Constraint (4) is kept and (6) is added. This is because the minimization of the maximum difference between the computed and desired values ensures the simultaneous minimization of both objectives [24], allowing to convert (3) into a single-objective optimization function (5).

$$\beta = \left\{max \left|\frac{RE-RE^d}{RE^d}\right|, \left|\frac{RCL-RCL^d}{RCL^d}\right|\right\} \tag{5}$$

Subject to (4) and

$$\begin{aligned} \beta &\geq \left|\frac{RE-RE^d}{RE^d}\right| \\ \beta &\geq \left|\frac{RCL-RCL^d}{RCL^d}\right| \end{aligned} \tag{6}$$

Internal analysis. This stage comprises the mathematical modeling required to derive the auxiliary models necessary for calculating the parameters of the conceptual model and for parameterizing the relationships that link process outputs (efficiency indicators and restricted functions) to inputs (coordination and decisions variables). This includes the specification of input data, parameters, and constants, *etc.*; the definition of calculation procedures for all output variables and restricted parameters (including their limits), and simulation and graphic representation. Through this process, the conceptual model is transformed into a detailed decision-making model.

In this contribution, the parameterization of the indicators was obtained thanks to an experimental plan and the simulation of the corresponding tests using the Aspen Plus software. The process performance was simulated for operating temperatures between 300 and 550°C, which are boundaries recommended in the literature for plastic pyrolysis. The efficiency indicators of the conceptual mathematical model were calculated for each test using the set of expressions given in Eq. (7).

$$
\begin{aligned}
FMT &= \sum_{i=1}^{nl} FM_i \\
ECL &= \sum_{i=1}^{nl} AE_i \\
AE_i &= FM_i * PCi \\
DL &= \sum_{i=1}^{nl} \frac{FM_i}{FMT} DL_i \\
VL &= ML \,/\, DL \\
EG &= \sum_{i=1}^{ng} FM_i PC_i \\
DG &= \sum_{i=1}^{ng} \frac{FM_i}{FMT} DL_i \\
VG &= MG/DG \\
EE &= (ME)(CCP)\Delta T \\
EO &= ECL + EG
\end{aligned} \tag{7}
$$

where subindex *i* refers to each individual substance in the liquid or gaseous phase; *FMT* is the total mass fraction of the liquid; n_l is the amount of liquid substances; *ECL* is the liquid fuel energy; AE_i is the energy contribution of liquid substance *I*; PC_i is the calorific value of liquid substance *I; DL* is the density of the liquid; *VL* is the volume of liquids; *ML* is the total mass of liquid obtained from the simulation; *EG* denotes the energy of the non-condensable gases; *ng* is the amount of gaseous (non-condensable) substances; *DL* represents the density of the gases; *MG* is the total mass of gas obtained from the simulation; *VG* denotes the volume of the gases; *EE* is the supplied energy; *ME* is the mass of the plastic input; *CCP* is the heat capacity of the plastic; ΔT represents the difference between the pyrolysis and ambient temperature; and *EO* denotes the obtained energy.

From the adopted conceptual mathematical model, the relationships selected for parameterization were *RE* (energy yield), *RCL* (liquid fuel yield), *PCL* (calorific power of the liquid fuel), and *PCG* (calorific power of the gaseous fuel), all of them as a function of the pyrolysis temperature *T*, as shown in Eq. (8).

$$
\begin{aligned}
RE &= (EE - EO) \,/\, ME \\
RCL &= VL \,/\, ME \\
PCL &= ECL \,/\, ML \\
PCG &= EG/MG
\end{aligned} \tag{8}
$$

The indicators given in Eq. (8) were processed as functions of the pyrolysis temperature *T* obtained through logarithmic-signomial models, as expressed in Eq. (9). The parameters of these models were obtained by adjusting a general nonlinear regression model from the data generated during the virtual experiments [29].

$$
y = a_0 + \sum_i b_i Ln\, x_i + \sum_j c_j \prod_i x_i^{\alpha_{ij}} \tag{9}
$$

where a_0, b_i, c_i, and α_{ij} are adjusted parameters, and *i* and *j* are indices of the independent variables and the equation terms, respectively.

The experimental data were processed by means of the Statgraphics package, which made it possible to obtain the logarithmic-signomial models for the selected performance indicators.

The solution of the optimization model was obtained using the Microsoft Excel Solver add-in. All the data were organized within Excel, dividing them into coordination variables, decision variables, efficiency indicators, desired values, restricted functions, and auxiliary data. The efficiency indicators (*RE* and *RCL*) were calculated using the nonlinear regression equations derived from the processed results of the virtual experiment.

Process simulation in Aspen Plus

Data acquisition for system analysis was performed through simulations performed in the Aspen Plus software using thermodynamic equilibrium approximations. It is well-known that real-world pyrolysis processes are predominantly kinetically limited rather than equilibrium-limited. Notwithstanding, the equilibrium model has yielded acceptable representations for simulating the thermochemical transformation of different types of plastics [14]. In these approximations, the Gibbs free energy minimization principle governs equilibrium modeling, considering that the reactor has its most stable composition when chemical equilibrium is attained, which occurs when the entropy increases and the Gibbs free energy is minimized. Equilibrium models serve as a benchmark for constructing reactors with a fair prediction of the final composition, as well as for monitoring process parameters, including pressure and temperature [27]. Thus, the thermodynamic model adopted herein could prove suitable as a preliminary approximation. A complementary study addressing a kinetic model is currently under development and is expected to provide a more accurate representation of the formation and distribution of the main pyrolysis by-products.

The process flow diagram shown in Fig. 3 and the associated model specifications were implemented following the recommendations reported in [14] and [28].

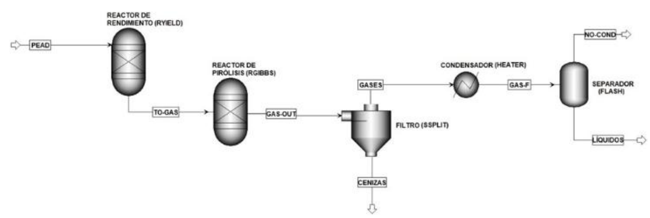

Figure 3. Flowchart for the simulation of waste plastic pyrolysis.
Source: Adapted from [14]

Modules or blocks

- RYIELD: performance reactor used to decompose waste plastics that allows for the transformation of a non-conventional solid to conventional components.
- RGIBBS: thermodynamic pyrolysis reactor through which chemical and phase equilibrium are determined.
- SSPLIT: stream splitter used as a filter where primary solids are recovered.
- HEATER: heat exchanger or condenser which allows pyrolysis gases to be cooled.
- FLASH: unit for separating liquid fuels and non-condensable gases.

Flows

- HDPE: inlet of high-density polyethylene as a non-conventional solid.
- TO-GAS: decomposition of HDPE into conventional components.
- GAS-OUT: exit gases resulting from pyrolysis.
- ASH: solid primary components.
- GASES: stream of gases to be cooled.
- GAS-F: cooled gases.
- LIQUIDS: liquid products obtained.

- NO-COND: non-condensable gaseous products obtained.

Main considerations or assumptions

i) Amount of initial raw material: 36.07 kg, according to the basic design of the installation.

ii) Temperature range: 300-550 °C, according to the virtual experimentation plan.

iii) Isobaric process at 1 atm.

iv) Simulation of feedstock pretreatment stages: collection, sorting, washing, drying, and shredding is not included.

v) All chemical reactions reach equilibrium inside the pyrolysis reactor (RGIBBS).

vi) Based on the literature and the selected feedstock, the formation of a significant amount of different substances can occur [14, 25]. Liquid products are anticipated to contain higher proportions of biphenyl, methylnaphthalene, phenanthrene, ethylbenzene, xylene, propylbenzene, methylpropylbenzene, benzene, toluene, styrene, alpha-methylstyrene, iso-propylbenzene, tetradecane, pentadecane, hexadecane, nonene, undecane, naphthalene, fluorene, indene, benzophenone, acetone, acenaphthene, acenaphthalene, and limonene, among others. For gases, the following are expected in greater proportion: methane, ethylene, propylene, ethane, propane, hydrogen, carbon monoxide, and carbon dioxide.

vii) At the exit of the process, the gases are cooled down to 30 °C (condensation temperature).

For the input of the feedstock (HDPE) into the model, the plastic was simulated as a non-conventional solid. This approach has proven effective for the Aspen Plus simulation of thermochemical processes involving solids as feedstock [14, 28]. The proximate and ultimate analysis data of the plastic (required for the simulation) were obtained from the literature [14] and are summarized in Table I.

Table I. Proximate and ultimate analysis of HDPE plastic

Proximate analysis	(% weight)	Ultimate analysis	(% weight)
Moisture	0.0	C	83.90
Fixed carbon	0.03	H	14.70
Volatile material	98.57	O	0.0
Ash	1.40	N	0.0

Source: Adapted from [14]

Results and discussion

The simulated composition of the liquid fractions resulting from the process, regardless of temperature, allowed identifying four major components (>98%): naphthalene ($C_{10}H_8$), phenanthrene ($C_{14}H_{10}$), benzene (C_6H_6), and toluene (C_7H_8). For this reason, the value of parameter *nl* in Eq. (7) was set at a value of 4. The gas or non-condensable phase resulting from the process was mainly (>98%) composed of methane (CH_4), ethane (C_2H_6), and hydrogen (H_2). This allowed setting the *ng* parameter of Eq. (7) at a value of 3.

The energy yield (*RE*) and liquid fuel (*RCL*) values, as well as the calorific value of the liquid fuel (*PCL*) and the non-condensable gases (*PCG*) shown in Table II, were calculated from Eq. (8) using data obtained from the execution of the virtual experiment plan.

Table II. Results of the virtual experiment for the selected indicators by changing the pyrolysis temperature *T*

T (°C)	RE (kJ/Kg)	RCL (ml/Kg)	PCL (kJ/Kg)	PCG (kJ/Kg)
300	42 689.72	12.32	37 965.62	49 048.96
330	42 619.83	12.32	37 971.34	49 009.95
360	42 543.78	12.35	37 905.34	48 984.56
400	42 424.73	12.36	37 935.40	48 892.50
430	42 331.76	12.40	37 921.45	48 786.90
450	42 255.11	12.40	37 935.87	48 701.50
480	42 128.96	12.44	37 934.16	48 553.49
500	42 031.06	12.47	37 923.64	48 442.83
550	41 730.12	12.57	37 904.69	48 129.48

Source: Authors

Approximation functions

The experimental data for each modeled indicator were processed using the Statgraphics software. The best-fit power relationships were identified through regression analysis between the logarithms of the output variables and *T*. In this way, multiple linear regression models were proposed to describe the relationship between each indicator and the terms resulting from the processing. The results for *RE, RCL, PCL*, and *PCG* are shown in Table III, Table IV, Table V, and Table VI**,** respectively, and the corresponding adjusted models in Eqs. (10) to (13). The specific functional form of each equation obeys the best fit found.

Table III. Analysis of variance for the energy yield (*RE*)

Source	Sum of squares	Df	Mean square	F-Ratio	p-value
Model	742 732	2	371366	144.11	0.0000
Residual	15 461.9	6	2576.98		
Total (Corr.)	758 194	8			

Source: Authors

- R-squared = 97.9607
- R-squared (adjusted for d.f.) = 97.2809
- Standard error of est. = 50.764
- Mean absolute error = 30.0385
- Durbin-Watson statistic = 1.18066 (P=0.0086)

The equation that describes the adjusted model for the energy yield *RE* is shown in Eq. (10).

$$RE = 3.96103x10^6 - 130132\ln(T) - 4.01291x10^6T^{-0.041} \tag{10}$$

Table IV. Analysis of variance for the liquid fuel yield (RCL)

Source	Sum of squares	Df	Mean square	F-Ratio	p-value
Model	0.0490434	2	0.0245217	161.80	0.0000
Residual	0.00090933	6	0.000151555		
Total (Corr.)	0.0499528	8			

Source: Authors

- R-squared = 98.1796
- R-squared (adjusted for d.f.) = 97.5728
- Standard error of est. = 0.0123108

- Mean absolute error = 0.00901746
- Durbin-Watson statistic = 1.44673 (P=0.0309)

Eq. (11) describes the adjusted model for the liquid fuel yield (*RCL*).

$$RE = 55.4151 + 0.00470815\ (T) - 36.439T^{0.035} \qquad (11)$$

Table V. Analysis of variance for the caloric power of the liquid fuel (*PCL*)

Source	Sum of squares	Df	Mean square	F-Ratio	p-value
Model	4337.85	5	867.57	11.59	0.0354
Residual	224.531	3	74.8438		
Total (Corr.)	4562.38	8			

Source: Authors

- R-squared = 95.0786
- R-squared (adjusted for d.f.) = 86.8764
- Standard Error of Est. = 8.65123
- Mean absolute error = 3.4585
- Durbin-Watson statistic = 2.41084 (P=0.6008)

Eq. (12) describes the adjusted model for the liquid fuel yield *RCL*. Since this variable presented an oscillating behavior, the oscillation period was included in the model.

$$PCL = 64127 + 26{,}3271\ (T) - 5731{,}78\ \ln(\mathrm{T}) + \\ + 0{,}306382\ \mathrm{T}\cos(\pi T/28) - 0\,.\,149527T^2 - \\ - 0{,}000648136T^2\cos\,(\pi T/28) \qquad (12)$$

Table VI. Analysis of variance for the caloric power of non-condensable gases (*PCG*)

Source	Sum of squares	Df	Mean square	F-Ratio	P-Value
Model	704928	3	234976	332.31	0.0000
Residual	3535.48	5	707.096		
Total (Corr.)	708463	8			

Source: Authors

- R-squared = 99.501
- R-squared (adjusted for d.f.) = 99.2015
- Standard error of est. = 26.5913
- Mean absolute error = 16.8826
- Durbin-Watson statistic = 11.7445 (P=0.0377)

Eq. (13) describes the adjusted model for the caloric power of non-condensable gases (*PCG*).

$$PCG = 123145 - 16.5035(T) + 2992.05\ln(T) - \\ - 101209T^{-0.028} \qquad (13)$$

Optimization of the operating regime

Given the nonlinear nature of the selected efficiency indicators and constrained functions, the resulting mathematical model is nonlinear. The Microsoft Excel Solver add-in was employed, using algorithms that include the generalized reduced gradient methods and an evolutionary algorithm. Experimentation with both methods showed that the former tends to converge to local minima, which is a natural result of the oscillating behavior of the *PCL* variable. For this reason, and in order to obtain solutions closer to the global optimum, the results produced using the evolutionary algorithm are presented. Given the multi-objective nature of the model used, a reasonable compromise between the *RE* and *RCL* indicators is required for the specific values of *PCL* and *PCG*, corresponding to desirable variable values of both indicators. One of the optimization results is presented in Table VII, which shows the desirable values of the efficiency indicators and the corresponding constraint functions.

Table VII. Optimization results

	Required	Calculated
RCL value	37 930	37 935.77
RE value	48 700	48 700.14
Target cell (min)	Desired	Calculated
β	12.57	12.358
Variable cells	42 689.72	42 466.95
Pyrolysis temperature T	Original value	Final value
RCL value	0.008441	0.006447
RE value	Original value	Final value
Target cell (min)	400	450.3

Source: Authors

Discussion

Compared with results predominantly reported in the specialized literature—based on the individual or combined use of physical experiments and process simulation tools, such as Aspen Plus, HYSYS, DWSIM, and CHEMCAD, as illustrated in [14] and [18]—, the results obtained in this study reflect the potential of applying systems analysis and synthesis, decision-making modeling, and multicriteria optimization to the problem of transforming waste plastics into synthetic fuels. These approaches allow developing optimization models to assist in the decision-making process of the operational tasks related to this transformation, such as Models (1)-(2) and (3)-(4).

In particular, modeling based on thermodynamic equilibrium makes it possible to determine the pyrolysis temperature that best satisfies the decision-maker's preferences. Notably, the optimal temperature (450.3°C) was obtained via a preliminary approximation using a thermodynamic model. Thus, by using a detailed kinetics-based model, a final optimal temperature could be acquired.

Conclusions

The results obtained support the hypothesis that operational decision-making tasks associated with the transformation of plastic into synthetic fuel should precede physical experimentation, thereby reducing time and research costs.

The development of synthetic fuel production technology requires pyrolysis followed by condensation of the resulting gases. The parameterization of the process requires mathematical modeling, including both descriptive modeling and the modeling of the associated decision-making process.

The mathematical modeling of the HDPE to synthetic fuel transformation process must be performed first under thermodynamic equilibrium conditions and subsequently under kinetic modeling conditions. Accordingly, the conceptual mathematical decision-making framework corresponds to each of these types of descriptive models. In both cases, virtual experiments and further data processing are needed to find the approximation functions required by each process type.

Among the available tools, Aspen Plus is well suited for performing the virtual experiments required for constructing the approximation functions of the performance indicators and the restricted functions of the conceptual mathematical model.

The decision-making modeling includes two objectives, *i.e.*, energy yield (*RE*) and liquid fuel yield (*RCL*), as well as two technological constraints: liquid fuel calorific value (*LCP*) and the non-condensable gas calorific value (*NGQ*). Satisfying decision-makers' preferences requires the iterative variation of the desirable values of both objectives and lowering the values of both caloric powers, which enables the identification of the optimal operating parameters.

Once the expected composition of liquid and gaseous fuels—corresponding to the pyrolysis temperature that provides a satisfactory compromise for the decision-makers' preferences—has been determined, it becomes necessary to move on to the solution of the detailed process of operation, which will be the focus of the authors' next work.

This study provides an initial framework for the multi-objective optimization of plastic waste pyrolysis temperatures, thus facilitating the transition towards the subsequent optimization of the operation of the process and facility design based on kinetic descriptive modeling.

Acknowledgements

We gratefully acknowledge the institutional support of the Universidad de Antioquia (Colombia) and Universidad Tecnológica de la Habana (Cuba) in the realization of this joint research.

CRediT author statement

José Raúl Suárez Cruz executed the methodology under the supervision of José Arzola Ruiz and conducted the background research. José Arzola Ruiz supervised the research and provided critical feedback. Rolando Barrera Zapata provided modeling and simulation assessments as well as critical feedback throughout the research. All three authors contributed with the manuscript writing.

Conflicts of interest

The authors declare no conflicts of interest.

Access to research data

The datasets generated and/or analyzed during this study are available from the authors upon reasonable request.

Statement on artificial intelligence

The authors did not use IAG. The authors take full responsibility for the contents of this publication.

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