

Methods and Validation Techniques of Chemical Kinetics Models in Waste Thermal Conversion Processes

Magdalena Skrzyniarz ¹, Marcin Sajdak ², Anna Biniek-Poskart ³, Andrzej Skibiński ³, Marlena Krakowiak ¹, Andrzej Piotrowski ⁴, Patrycja Krasoń ¹ and Monika Zajemska ^{1,*}

¹ Faculty of Production Engineering and Materials Technology, Czestochowa University of Technology, 19 Armii Krajowej Ave., 42-200 Czestochowa, Poland; magdalena.kocyba@pcz.pl (M.S.); marlena.krakowiak@pcz.pl (M.K.); patrycjakrason01@gmail.com (P.K.)

² Center of New Technologies, Department of Air Protection, Faculty of Energy and Environmental Engineering, Silesian University of Technology, 22 B Konarskiego Ave., 44-100 Gliwice, Poland; marcin.sajdak@polsl.pl

³ Faculty of Management, Czestochowa University of Technology, 19 B Armii Krajowej Ave., 42-200 Czestochowa, Poland; a.biniek-poskart@pcz.pl (A.B.-P.); andrzej.skibinski@pcz.pl (A.S.)

⁴ Faculty of Mechanical Engineering and Computer Science, Czestochowa University of Technology, 42-200 Czestochowa, Poland; andrzej.piotrowski@pcz.pl

* Correspondence: monika.zajemska@pcz.pl

Abstract: This article discusses the potential of using computer-simulation methods in processes such as thermal waste conversion, i.e., pyrolysis, gasification, combustion and torrefaction. These methods are gaining in importance, among others, due to the difficulties in execution and high costs associated with conducting experimental research in real conditions or the need to obtain detailed data on the phenomenon under study in a relatively short time. Computer simulation also allows for numerous errors to be avoided, such as those that may occur during optimization activities, the effects of which may have serious consequences, both economic and environmental. In addition to their many advantages, the limitations and disadvantages of using computer-simulation methods were also indicated, mainly related to the interpretation and validation of the results obtained using modelling. Owing to the complexity of the phenomena occurring during thermal conversion, special attention was focused on models based on chemical kinetics, thanks to which it is possible to predict the quantitative and qualitative composition of products in these processes. The aim of this research is to identify the research gap in the field of issues related to models of chemical kinetics of thermal waste conversion processes.

Keywords: simulation; circular economy; sustainable development; waste; thermal conversion; kinetic model



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1. Introduction

Efforts are being made worldwide to promote the energy use of waste through combustion [1], gasification [2], pyrolysis [3] and torrefaction [4] as a strategy that fits, among others, into the idea of a circular economy [5,6]. These activities focus on finding sustainable alternatives for the effective use of waste, which loses the status of “rubbish” and becomes a valuable raw material for other processes [1]. Unfortunately, due to the heterogeneity of waste and the complexity of the phenomena occurring during thermal conversion, there are a number of limitations to its widespread use [7].

The European Union strongly supports activities aimed at preventing waste and reusing products. According to the EU Landfill Directive, by 2035, EU countries must limit the amount of municipal waste sent to landfills to 10% or less of the total municipal waste generated [8]. This creates an opportunity to manage waste that has previously been stored in landfills. Currently, the EU places great emphasis on increasing the share of recycling in waste management methods and reducing the share of landfilling [9].

Examples include two neighboring countries: Poland and Germany. Both countries are striving to transition their economies to a circular economy. In this respect, Germany is considered to be a country that has made a number of far-reaching changes to achieve this goal. Currently, 79% of all waste generated in Germany (64% of municipal waste) is recycled (data from Statistische Bundesamt). In Poland, 36.3% of all waste generated (26.7% of municipal waste) was recycled in 2022—according to data from the Central Statistical Office (called GUS in Poland). Both countries mentioned above have a similar hierarchy of waste management (Figure 1).

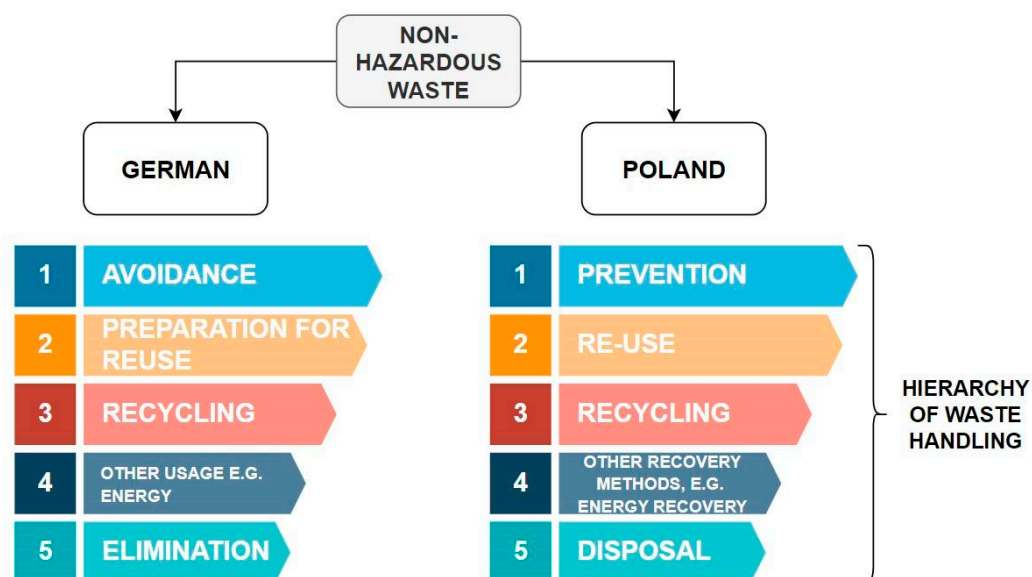


Figure 1. Hierarchy of treatment of non-hazardous waste [9,10].

Germany has introduced the “Principles for Sustainable Waste Management”, which contributes to the elimination of waste. These rules specify that the producer is responsible for each waste produced (also financially—“the polluter pays”). This encourages manufacturers to create new products responsibly. The “precautionary principle” allows for intervention in areas where general regulations do not function adequately. The “principle of proximity” requires that waste be disposed of as close as possible to the place of its generation, which does not exclude the export of waste if it is economically profitable. The “principle of subsidiarity” determines who will deal with waste management, taking into account factors such as transport costs, efficiency and benefits resulting from the proximity of the place of waste production and processing [11]. A special group of waste is chemical waste that, due to its properties (flammability, explosiveness, toxicity and others), is classified as hazardous waste [12–14] and requires proper handling [15], with particular care. Chemical waste includes waste oils [16], waste-containing asbestos, medical and veterinary waste, expired plant protection products and household chemicals [17]. As numerous scientific works indicate, hazardous waste is the most difficult waste to manage because, in the process of its thermal processing, it produces, among others, heavy metals and dioxins. Governments around the world are making a number of efforts to better manage and deal with hazardous waste. An example is Portugal. Over the last decades, the Portuguese government has introduced numerous solutions, such as the modification of the legal framework, creation of a network infrastructure that includes integrated systems of industrial waste treatment (ISIWT) and also development of new organizational methods to make the waste management system more effective [16].

Widely developed computerization addresses these problems by proposing numerical-simulation methods as an important tool in the analysis of complex chemical and gasodynamic phenomena occurring during the thermal conversion of waste [18,19]. The interest in using computer-simulation methods in thermal waste conversion processes is evidenced

by numerous scientific publications [20,21]. Using the popular science mapping tool VOSviewer (version 1.6.20) [20–23], an analysis was carried out using the Scopus database.

The datasets prepared on the basis of the Scopus database include an analysis of global literature on research topics focusing on chemical kinetics in relation to thermal conversion of waste. The research was performed in May 2024. The results of the literature analysis are based on the use of keywords and restrictions introduced in the advanced search in the Scopus database. In order to limit the number of documents found, only the titles of articles were analyzed (not abstracts and keywords). The search with the use of the string “TITLE-ABS-KEY” resulted in finding over a thousand documents that were not necessarily connected with the analyzed subject matter. The used string was as follows: TITLE ((“chemical kinetics” OR “chemical models” OR “kinetics model” OR “kinetic theory” OR “kinetics” OR “kinetic modeling”) AND (“waste”) AND (“thermal conversion” OR “gasification” OR “combustion” OR “torrefaction” OR “pyrolysis”)) AND PUBYEAR > 2018 AND PUBYEAR < 2026 AND (LIMIT-TO (SRCTYPE, “j”)). The number of results found was 212 documents. The timeframe was limited to the last six years, and the searching formula was limited only to article titles that appear in journals. Then, the results selected from the Scopus database were exported as CSV files and supplied into the VOSviewer program in order to analyze the correlations of the obtained literature list for a given subject area. The observed dependencies and relationships between the selected keywords required the creation of several datasets. Visualizations in the form of a map were created using the VOSviewer 1.6.18 software. As part of the attempt to interpret the keywords, the following approach was taken: the type of analysis was “co-occurrence”, the unit of analysis was “All keywords”, and the counting method was “Full counting”. The “minimum number of occurrences of a keyword” was set to six. This led to 142 results as those that “meet the threshold” among 2005 keywords. If the minimal number of occurrences of a keyword was five, the results that meet the threshold were 175. If that number was seven, it led to 107 results, and if the number was eight, the number of results was 89. Two of all the keywords were eliminated due to the lack of their importance to the subject matter, and they were “article” and “priority journal”. Figure 2 as well as Figure 3 show that the most frequently appearing words were kinetics, activation energy and pyrolysis with the total link strength of 1571, 1570 and 1561, respectively. However, the ranking of a keyword’s total link strength may differ a bit from that of their occurrences.

Selected	Keyword	Occurrences	Total link strength
☒	kinetics	141	1571
☒	activation energy	137	1570
☒	pyrolysis	144	1561
☒	thermogravimetric analysis	81	943
☒	reaction kinetics	63	793
☒	biomass	52	614
☒	thermogravimetry	36	597
☐	article	33	583
☒	kinetic parameters	37	487
☒	pyrolysis kinetics	45	451
☒	heating	26	398
☒	copyrolysis	26	354
☒	waste incineration	29	332
☒	fourier transform infrared spectroscopy	21	311
☒	temperature	20	308
☒	thermodynamics	21	298
☒	co-pyrolysis	28	293
☒	decomposition	16	281
☒	controlled study	14	277
☒	priority journal	14	276

Figure 2. Screenshot of top 20 keywords indicated by the VOSviewer with their number of occurrences and total link strength.

Among a total number of 2005 keywords, there were three that appear with a frequency of over 130 times; one keyword with a frequency of over 80, 60, 50 and 40 times each; and seven keywords with a frequency of over 20 times.

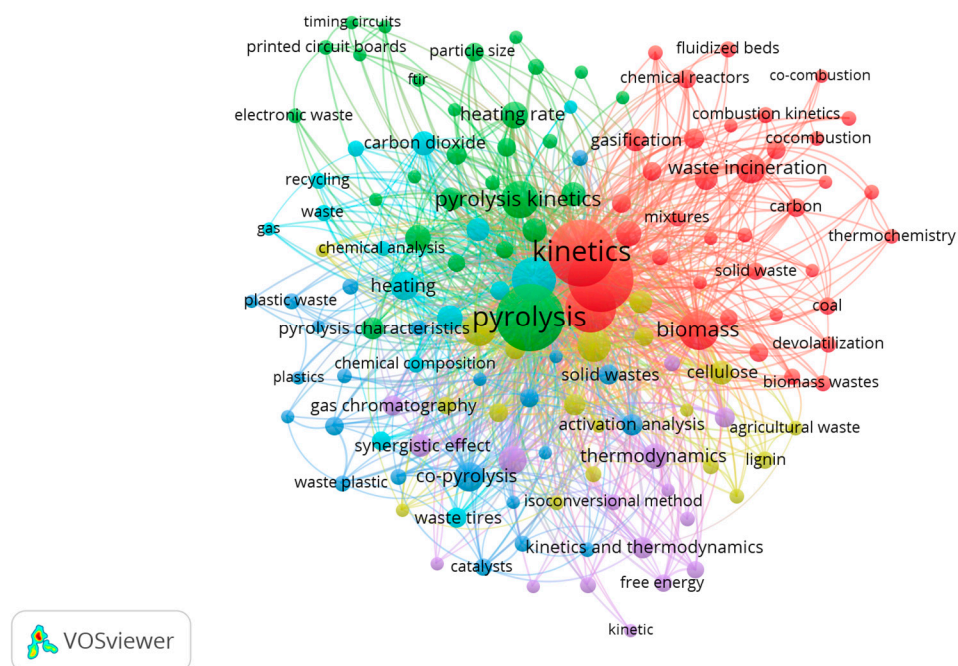


Figure 3. VOSviewer network visualization of keyword co-occurrence.

Using the VOSviewer software, the correlation between particular keywords that appear in documents being analyzed can be identified and presented as a map. The words are grouped into clusters to show their relationship. The size of the circles is positively correlated with the occurrence of the keywords. The more often a keyword appears, the larger the font size and circles. The strength of occurrences is indicated by the size of the nodes, while the strength of the relationships reflects the thickness of the lines between the nodes. The analysis shows that five clusters were identified in the network (red, green, blue, purple and yellow). The red cluster is connected with the keyword “kinetics” that indicates 139 links, “activation energy” with 139 links, “thermogravimetric analysis” with 136 links, as well as “biomass” indicating 121 links and “waste incineration” with 102 links. The green cluster refers to the keyword “pyrolysis”, indicating 137 links, correlated with “pyrolysis kinetics”. The connectivity included in the blue, purple and yellow clusters is less dominant, which is presented by the size of their circles.

Analyzing the “network” visualization, it was observed that, over the years, interest in chemical kinetics in the thermal conversion of waste processes has been growing. This is confirmed by the network of connections within the clusters. The keyword maps clearly indicate the high importance of the research topic undertaken, emphasizing the need to expand research in this area, especially in the context of predicting the chemical composition of thermal waste conversion products using chemical kinetics models. The analysis shows that, despite many scientific works published on this topic, there is still a research gap in the issues discussed in the article. With a view to promoting a sustainable development strategy around the world in which the effective use of waste (with diverse properties and elemental composition) plays an important role, there is an urgent need to develop mathematical models that take into account the chemical kinetics of thermal waste conversion. The use of computer-simulation methods in the analysis of complex thermal decomposition processes will assess their energy suitability and the environmental effects of their use.

2. Theoretical Background

2.1. The Essence of Computer Simulations

As a result of the development of technology, computer-simulation methods have been gaining importance in recent years, being used not only in many industries but also in business and government institutions [24]. Simulation takes various forms from

modelling simple systems and systems for operational management purposes, such as production and finance, to modelling complex systems for corporations, the global economy or environmental organizations [25,26]. In the initial stages of the development of simulation methods, simulations were used primarily in the natural, technical and economic sciences [23,26,27]. They are currently widely used on a wide scale in various industries, such as the automotive industry [25,28] (Nissan, PSA Peugeot Citroën, Toyota, Ford Motor Company) and fields of science, in particular global scientific and research centers [29] (the Universities of Michigan, Tokyo, Minnesota, Karlsruhe and Colorado) as well as by the National Aeronautics and Space Administration (NASA) [30–32]. Currently, there is even a trend of the overuse of computer-simulation methods, which can be explained not only by the degree of development of science but also by the ease and universality of their usage. The appropriate use of computer-simulation methods may be determined by many factors, in particular [23,33] the following:

- Too high costs of conducting experimental research in real conditions;
- The need to quickly obtain accurate data on the phenomenon under study;
- The need to obtain a range of information that is impossible to obtain exponentially, which will complement and enrich the existing state of knowledge;
- The need to avoid mistakes whose consequences may be serious;
- The lack of an actual research object or when it is only at the design stage.

Numerical models typically consist of input data, decision variables and output data (Figure 4) [34–37]. Input data introduce constant values into the model for a single experiment, while decision variables are variables controlled by the researcher. The output data are determined by the input and decision data; they enable the selection of a certain combination of decision variable values that is best from the point of view of the analyzed problem.

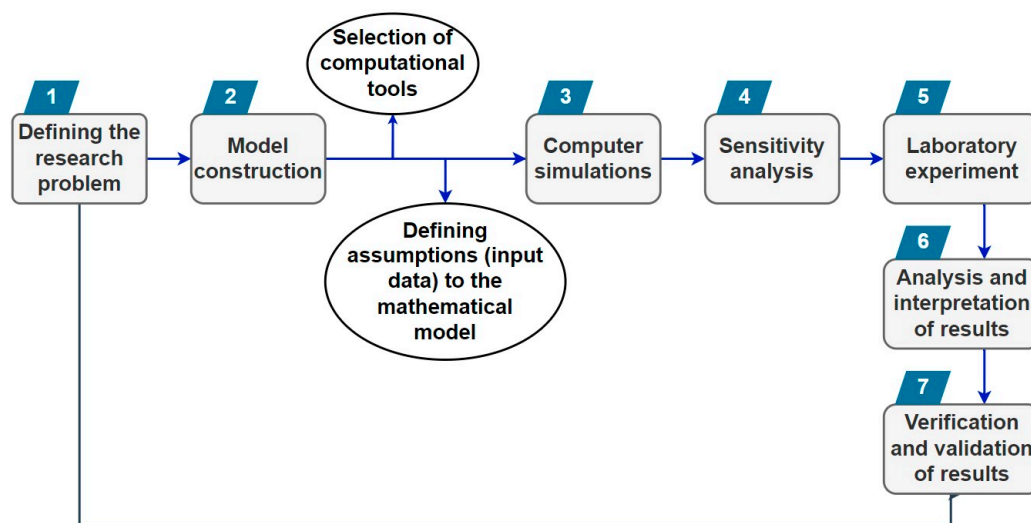


Figure 4. Stages of computer simulation [33].

The greatest advantage of computer simulations is the ability to analyze various time periods with a full picture of the phenomena occurring at each stage of the analyzed process. This is extremely difficult or even impossible to observe in real conditions. A great advantage of simulation is also the repeatability of processes because, once the model has been developed, it can simulate the process any number of times. In addition, the model can incorporate various variants, such as forcing, interference and other changes. The cost of building a model is, in many cases, much lower than conducting research in real conditions, and the possibilities of interpreting the results increase with the number of recorded parameters. However, it is important to note that both the design and interpretation of simulation results require experience and skills to include all relevant parameters and

variables for a given process in the simulated problem. Therefore, the main disadvantage of computer simulations is the possibility of making an error when creating the model and the difficulty in properly interpreting the simulation results. These issues are caused by the human factor since a person creates the simulation model and may incorrectly formulate the simulated problem and adjust the tool as well as draw incorrect conclusions from the simulations (Figure 5) [38–40].



Figure 5. Motivation, advantages and disadvantages of computer simulations [21,33,39,40].

2.2. Application of Numerical-Simulation Methods in the Analysis of Thermal Conversion Processes of Fuels and Waste

As numerous scientific works indicate, the main way to produce cleaner energy [41,42], especially in the era of energy transformation and decarbonization [43], is to employ thermal

conversion processes such as pyrolysis [44–46], combustion [47–49], gasification [50–54] or torrefaction [55,56]. The input material in the above-mentioned processes includes not only commonly used biomass [18,57,58] but also various types of waste [59,60], including plastics (e.g., PP, PET, PE) [61–64], municipal solid waste (MSW) [65], waste from the recycling of scrap tires [66,67], rural domestic waste [68] and refuse-derived fuel (RDF) [69–72] and solid recovered fuel (SRF) [73]. The initial stage of both combustion and gasification is pyrolysis [74,75].

Numerous scientific and research centers are attempting to increase the share of waste in energy production through thermal conversion [76,77]. However, providing a comprehensive description of thermal degradation is highly problematic due to the complexity of these processes [18,78,79]. The urgent need to understand and optimize these processes [80] has contributed in recent years to intensive development in the elaboration of numerical models [81,82], and the main research efforts are focused on understanding the reaction mechanisms of the kinetics of thermal conversion processes [83–85]. Chemical kinetics is crucial in comprehending the complex chemistry of the reactions of these processes and the creation of mathematical models [86–89].

Thermal conversion processes can be simulated using three different approaches:

- i. Computational fluid dynamics models [47,90–93];
- ii. Kinetic models [18,94,95];
- iii. Equilibrium models [52,96–98].

Equilibrium models are generally easy to implement, among others, due to numerous simplifications [99] (Figure 6). Depending on the method used to calculate chemical equilibrium, equilibrium models can be classified into two categories:

- i. Stoichiometric models;
- ii. Non-stoichiometric models.

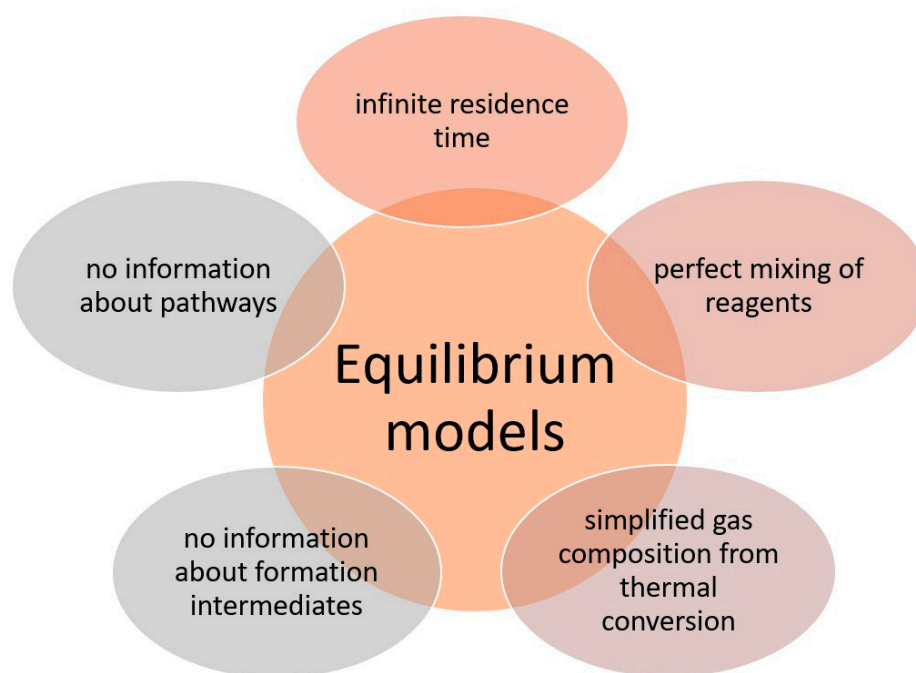


Figure 6. Simplifications of equilibrium models [99].

In stoichiometric models, the equilibrium is determined by using equilibrium constants for each reaction involved in the analyzed process. In contrast, in non-stoichiometric models, it is determined by minimizing the Gibbs free energy [38].

Kinetic modelling is quite complex [100], and the models are divided into the following:

- Lumped models [75,101,102];
- Other distributed kinetic models [103–107].

Most of the models described in the literature are simplified models that only allow for the prediction of the char yield and degassing time [108,109]. Unfortunately, this approach is not sufficient. From the energetic point of view of thermal conversion processes, it is extremely important to provide information on the temperature distribution, kinetic parameters and chemical composition of the gases released during the above-mentioned processes [98,110]. Although these issues have been extensively studied both theoretically and experimentally using various techniques, they still require more attention and research [111–113]. Thermal analysis techniques, such as (TG) [107], (DSC), (DTA), FTIR [114], MS or various combinations thereof, i.e., (TG–FTIR) [115], (TG–MS) or (TG–MS–FTIR), are considered effective techniques for examining the thermal degradation of both fuels and waste. The above-mentioned techniques provide information about the analyzed processes, enabling a better understanding of them, and above all, they can constitute input data for computer simulations [116–118].

Table 1 lists the thermal conversion processes in which computer simulations were employed.

Table 1. Use of computer simulations to predict products of thermal conversion of biomass.

Process	Feedstock Type	Kinetic Mechanism	Res.
Pyrolysis Single-step and multi-step thermos kinetic study multi-step mechanism reaction	Biomass: grass <i>Eleusine indica</i>	Eleusine indica $\left\{ \begin{array}{l} \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[119]
	Kinetic triplets	Catole coconut $\left\{ \begin{array}{l} \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[120]
	Butia seed waste (BSW)	BSW $\left\{ \begin{array}{l} \text{Extractives} \xrightarrow{k_e} \text{Volatiles} + \text{Char} \\ \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[121]
	Pecan nutshell	PNS $\left\{ \begin{array}{l} \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[122]
	Macauba endocarp (<i>Acrocomia aculeate</i>)	Macauba endocarp $\left\{ \begin{array}{l} \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[123]
Pyrolysis	Royal palm tree waste	(Royal palm tree waste) $\left\{ \begin{array}{l} \text{Extractives} \xrightarrow{k_e} \text{Volatiles} + \text{Char} \\ \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[124]
Pyrolysis	Poplar and eucalyptus wood sawdust	The kinetic parameters were computed via model-fitting (inflection point and multiple linear regression) and model-free (OFW and KAS) methods.	[125]
Thermal conversion	<i>Bambusa vulgaris</i> dust (BD) and <i>delonix regia</i> pods peels (DRP)	Model-free methods, like Kissinger–Akahira–Sunose (KAS) and Flynn–Wall–Ozawa (FWO), were applied for the determination of kinetic parameters.	[126]
Pyrolysis	<i>Sesbania bispinosa</i>	The three-pseudo-component model is made up of hemicellulose, cellulose and lignin. Artificial neural networks (ANN) are models based on the operation of the human brain.	[104]

Table 1. Cont.

Process	Feedstock Type	Kinetic Mechanism	Res.
Combustion	Biomass	Cellulose, hemicellulose, lignin, biomass $\xrightarrow{1}$ Active intermediate $\xrightarrow{2}$ Volatiles $\xrightarrow{4}$ Gas $\xrightarrow{3}$ Y Char + (1 - Y)Gas (1) Biomass → Tars (2) Biomass → Volatiles (3) Biomass → Char (4) Tars → Volatiles (5) Tars → Char (6) Char + O ₂ → CO ₂ (7) Char + CO ₂ → 2 CO (8) Char + H ₂ O → CO + H ₂	[48]
Pyrolysis		Mango seed waste $\left\{ \begin{array}{l} \text{Extractives} \xrightarrow{k_e} \text{Volatiles} + \text{Char} \\ \text{Hemicellulose} \xrightarrow{k_h} \text{Volatiles} + \text{Char} \\ \text{Cellulose} \xrightarrow{k_c} \text{Volatiles} + \text{Char} \\ \text{Lignin} \xrightarrow{k_l} \text{Volatiles} + \text{Char} \end{array} \right.$	[127]
Pyrolysis	Virgin	Cellulose, hemicellulose, lignin (Virgin biomass) $\xrightarrow{k_1}$ Active biomasse $\begin{cases} \xrightarrow{k_3} (1-Y)\text{Gas} + Y\text{Biochar} \\ \xrightarrow{k_2} \text{Tar} \end{cases}$ $\xrightarrow{k_4}$ Tar	[128]
Pyrolysis three-independent parallel reactions model	Beech wood, Rice husk	A three-independent-parallel-reactions model is used to model the kinetics of total devolatilization.	[75]
The two-step kinetic model proposed by Koufopoulos et al. for lignocellulosic biomass pyrolysis	Wood sawdust, bagasse, peanut hull, douglas fir bark, and rice husk		[129]
Torrefaction process	Beechwood	- lump kinetic scheme; - detailed kinetic scheme developed by Andr�es and Ingwald; - detailed kinetic scheme developed by Debiagi et al. with a one-dimensional model.	[130]
Pyrolysis		Wood $\begin{cases} \xrightarrow{k_C} \text{Char} \\ \xrightarrow{k_L} \text{Tars} \\ \xrightarrow{k_G} \text{Gas} \end{cases}$ $k = k_C + k_L + k_G$ One-component mechanism of primary wood pyrolysis proposed by Shafizadeh and Chin. Multi-component (or multi-stage) mechanisms of wood/biomass pyrolysis.	[131]
Pyrolysis	Biomass	(A) Cellulose $\xrightarrow{k}$ tar + coal + gasext (B) Hemicellulose $\begin{cases} \xrightarrow{k_{11}} 0.063 \text{ volatile matter I} \\ \xrightarrow{k_{12}} 0.117 \text{ volatile matter II} \end{cases}$ + 0.820 solid intermediate I $\xrightarrow{k_2}$ 0.310 volatile matter + 0.690 solid intermediate II $\begin{cases} \xrightarrow{k_{31}} 0.900 \text{ volatile matter} \\ \xrightarrow{k_{32}} 0.300 \text{ gases} + 0.610 \text{ coal} \end{cases}$ (C) Lignin $\begin{cases} \xrightarrow{k_{11}} 0.300 \text{ volatile matter I} \\ \xrightarrow{k_{12}} 0.100 \text{ volatile matter II} \end{cases}$ + 0.600 solid intermediate $\begin{cases} \xrightarrow{k_{21}} 0.090 \text{ volatile matter} \\ \xrightarrow{k_{22}} 0.300 \text{ gases} + 0.610 \text{ coal} \end{cases}$	[126]
Combustion	Polyethylene	A Non-isothermal 1D model	[132]
Gasification process	Pine sawdust	Comprehensive model was developed by Aspen Plus.	[133]
Pyrolysis	Wood, grass, and crops	Chemical reaction neural networks (CRNN) model	[58]

Table 1. Cont.

Process	Feedstock Type	Kinetic Mechanism	Res.
Pyrolysis	Biomass	Two-stage semi-global mechanism (CFD) <i>Primary reaction</i> <i>Secondary reaction</i>	[134]
Gasification		Main kinetic schemes for wood gasification: (1) Wood $\rightarrow \begin{cases} \text{Gas} \\ \text{Tar} \\ \text{Char} \end{cases} \rightarrow \text{Tar} \rightarrow \begin{cases} \text{Gas} \\ \text{Char} \end{cases}$ (2) Cellulose $\rightarrow$ Cellulose Active $\rightarrow \begin{cases} \text{Tar} \\ \text{Char} + \text{Gas} \end{cases} \rightarrow \text{Tar} \rightarrow \text{Gas}$ (3) Virgin Biomass $\rightarrow \begin{cases} \text{Volite} + \text{Gases} \\ \text{Char} \end{cases} \rightarrow \begin{cases} \text{Volite} + \text{Gases} \\ \text{Char} \end{cases}$	[51]
Pyrolysis	Polietylen, polipropylen, politereftalan etylenu		[116]
Pyrolysis	Empty fruit bunch	A simplified first-order gasification reaction model	[135]
		Virgin Biomass (Cellulose, Hemicellulose, Lignin) $\xrightarrow{k_1}$ Active Biomass (solid phase) $\xrightarrow{k_2, k_3}$ (1-v) Gas (gas phase) + Biochar (solid phase) + Bio-Oil Vapours (gas phase)	[136]
Torrefaction	Willow		[86]

According to the analysis, researchers have most often used the equation describing the relationship to explain the phenomena occurring during the thermal conversion of biomass and, in particular, pyrolysis (1) [104]:

$$\text{Biomass (SB)} \xrightarrow{K(t)} \text{Volatile(condensable + non condensable)} + \text{Biochar} \quad (1)$$

Che et al. [137] noted that Huazhong University of Science and Technology State Key Laboratory of Coal Combustion made significant advancements in the numerical simulation of gasification technology. Yang Haiping utilized the HSC chemistry package and the PSR reactor model to simulate the thermodynamic equilibrium and dynamic equilibrium of the palm oil waste pyrolysis process. The results obtained by Haiping revealed that the initial products contain significant amounts of H_2 , CO , CO_2 , CH_4 , H_2O and coke and small amounts of C_2H_2 , C_2H_6 , C_3H_8 and others in addition to the concentrations of H_2 and CO , which grow with the rise in the pyrolysis temperature.

Noteworthy are the computer simulations conducted by Peters et al. [138], who modelled the biomass pyrolysis process using an innovative reaction model in the Aspen Plus (version v14) program. This model was based on the three main building blocks of woody biomass, namely cellulose, hemicellulose and lignin. The pyrolysis process was described using 149 reactions. The linear regression algorithm took into account secondary pyrolysis reactions, enabling the calculation of slow and intermediate pyrolysis reactions. The model of bio-oil included chemical compounds, such as organic acids, aldehydes, alcohols, ketones, phenols, sugar derivatives and degraded lignin, and the produced carbon was modelled implementing the actual elemental composition.

A diagram of the reaction mechanism employed by Petersen et al. is presented in Figure 7 [138].

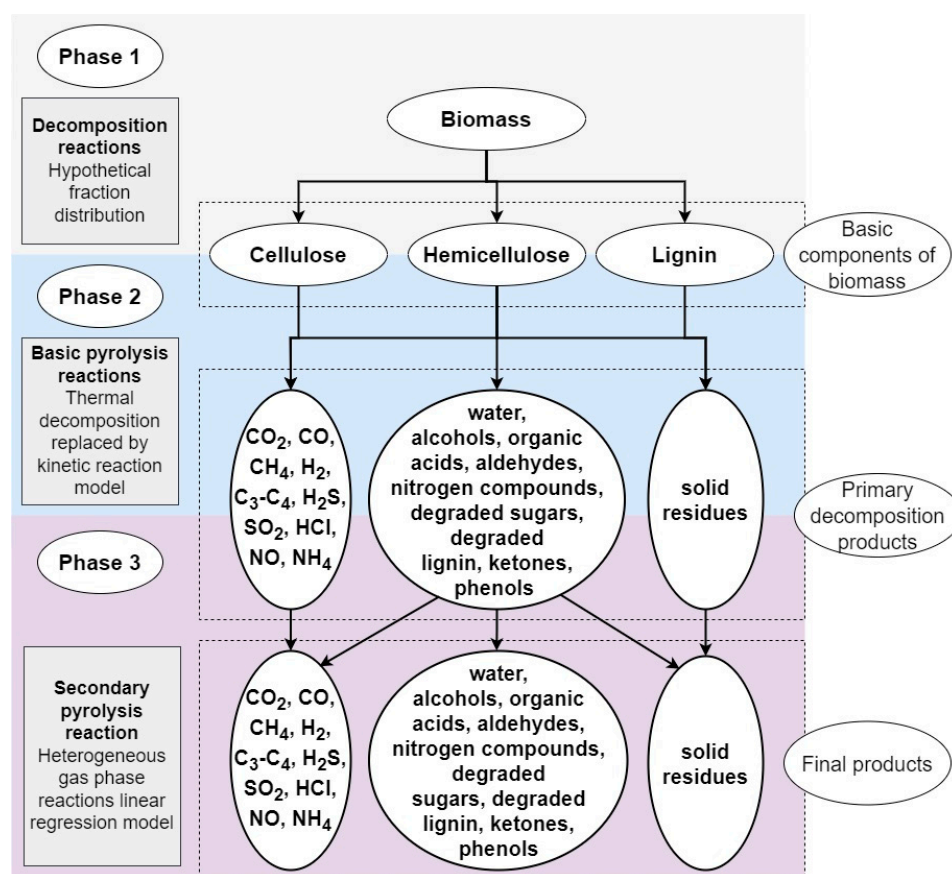


Figure 7. Three-stage pyrolysis reaction diagram [138].

The above model takes into account primary pyrolysis reactions as well as secondary cracking reactions. The pyrolysis mechanism was divided into three phases, namely one decomposition phase and two pyrolysis phases. The first phase is a virtual reaction step that breaks down the biomass into three main biochemical building blocks: cellulose, hemicellulose and lignin. During the second phase, the decomposition and volatilization of biomass fragments took place, leading to high efficiency of the liquid fraction. This is the dominant reaction mechanism for fast pyrolysis processes with short gas residence times. The third phase involved secondary cracking and charring reactions, which increased the gas and carbon yields at the expense of liquid yields as a consequence of secondary (catalytic) cracking reactions. These reactions are more significant with the increasing residence time and are, therefore, particularly important for slow and intermediate pyrolysis reactions. Petersen et al. [138] proposed a model that allows for the simulation of fast and slow pyrolysis of any lignocellulosic raw material with a known composition [138]. Moreover, a predictive and detailed modelling approach enabled a comprehensive assessment of

the properties of bio-oils obtained from various types of lignocellulosic biomass under various pyrolysis conditions (including fast and slow pyrolysis). Peters et al. emphasize that, to date, the analysis of pyrolysis processes has been based on simple models with a very simplified composition of bio-oil. The authors point out that their work is the first to present a comprehensive kinetic model of the reaction, which can be easily implemented in Aspen Plus and similar thermal conversion simulation software packages.

A similar approach was proposed by Granados et al., who modelled the biomass torrefaction process consisting of the three stages previously described in Petersen's work [139]. The process starts with drying the biomass to remove moisture, followed by heating the completely dry biomass. When the temperature grows, the biomass degassing process begins, resulting in the formation of condensable and non-condensable volatile substances and a solid residue. At low temperatures, the hemicellulose decomposition rate is high and dominates the entire torrefaction process. Only at high temperatures do some of the cellulose and lignin also begin to decompose but to a lesser extent. After primary degassing, secondary reactions occur where the produced condensable volatiles can react and form new solid and volatile components [139].

Park et al. [140] proposed a simplified approach to modelling the thermal conversion of biomass. Using Aspen Plus (version 14.3) software, they modelled the impact of the process operating conditions on biomass torrefaction using a one-dimensional reactor. The input data for the modelling were taken from the literature, and the diagram of the kinetic mechanism is presented in Figure 8. The results obtained by Park et al. confirmed that the energy efficiency of the torrefaction process increases with temperature (Figure 8).

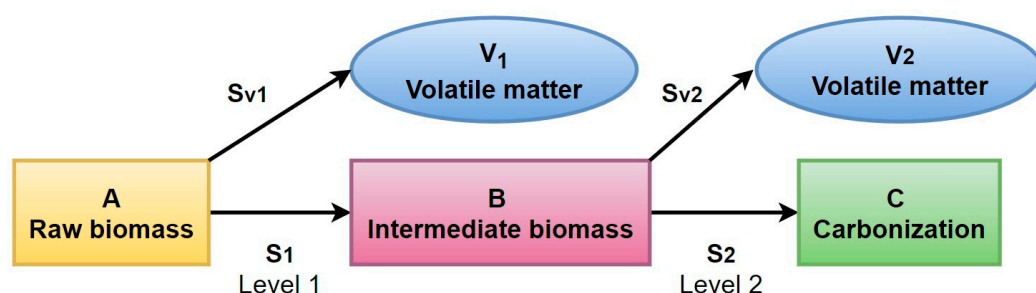


Figure 8. The scheme of chemical reaction kinetics mechanism proposed by Park et al. [140].

Yet another approach was proposed by Bates et al. [141], who developed a kinetic model for estimating the torrefaction products. The model is based on the mechanism originally proposed by Di Blasi and Lanzetta for the degradation of pure hemicellulose. Oliveira et al. [142] developed a kinetic model of the solid waste gasification process. The proposed mathematical model allowed for the detailed analysis of the processes occurring during gasification, taking into account partial derivatives, through the use of a CFD tool.

Also noteworthy is the approach to modelling the thermal conversion of biomass proposed by Wang et al. [126]. The authors developed a model for predicting pyrolysis products based on the Coats–Redfern method and the Kissinger method (Figure 9).

Yet another approach to simulating the biomass gasification process was proposed in the work by Gambarotta [42], who used a non-stoichiometric equilibrium model in downdraft gasifiers. The author utilized a five-component composition of the raw material for the calculations, i.e., forest waste (carbon, hydrogen, oxygen, nitrogen and sulfur), and included fifteen chemical compounds for the synthesis gas. The model calculated the relative amounts of gasification products and the calorific value of the synthesis gas. Gambarotta emphasized that the advantage of the non-stoichiometric approach is that it can easily calculate not only the concentrations of the main gasification products but also the concentrations of the by-products, especially chemical compounds containing nitrogen and sulfur. At the same time, he pointed out one of the main disadvantages of equilibrium models, namely the overestimation of molecular hydrogen and the underestimation of methane. The model developed by Gambarotta was analyzed for the sensitivity of the

influence of the selected parameters on the process and then verified by comparing the obtained simulation results with experimental data found in the literature. The model occurred to be effective in simulating the biomass gasification process with an acceptable level of error.

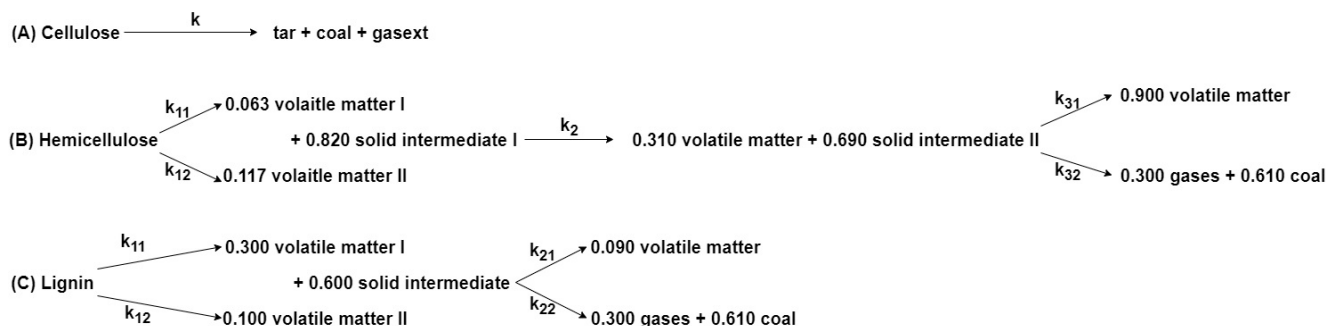


Figure 9. Model according to Wang et al. [126].

The actual reaction patterns of waste pyrolysis, including biomass and plastics, are extremely complex due to the formation of over one hundred intermediate products [117,143,144]. RDF is a special type of waste that is more complex than biomass due to its heterogeneous nature [72]. The amount of research on the kinetic modelling of RDF is much smaller compared to other fuels [71,145,146]. Three different approaches have been used in the literature to model the kinetics of thermal degradation of complex solid fuels, such as RDF. The first one considers fuel as one homogeneous species. The second approach considers the RDF pyrolysis rate as a weighted sum of the pyrolysis rates of cellulose, lignin, hemicellulose, polyethylene and other plastics. The third approach, similar to the second, considers the RDF pyrolysis rate as the weighted sum of the pyrolysis rates of paper, cardboard, wood, polyethylene and other plastics. The second and third approaches assume that possible interactions between the RDF components have a negligible impact on pyrolysis [71,146].

The research conducted by Zhou et al. [144] deserves attention. The authors developed a model to describe the heat transfer processes inside a porous RDF particle composed of polyethylene and cardboard. The model also considers the heat of the fusion of polyethylene (PE). To describe the degradation of polyethylene and cardboard, the authors adopted a one-stage global model and a scheme of two consecutive first-order reactions. To match the results of experimental research, the authors selected and modified two widely used heat transfer models—the Kunii and Smith model and the Breitbach and Barthels model. Moreover, they investigated the influence of the heat transfer model on the prediction of the RDF pyrolysis process. The authors achieved a high level of agreement between the results obtained through modelling and the experimental results for both the modified Kunia and Smith model and for the Breitbach and Barthels model.

On the other hand, Çepelioğullar et al. [146] modelled the pyrolysis process of RDF fuel in four reaction stages. The authors observed that the thermal decomposition of RDF involved many stages, which consisted of the decomposition of cellulose and plastics. Similarly, Bosmans et al. [147], using MATLAB (version R2023a) software, modelled the RDF fuel pyrolysis process, assuming four independent, parallel first-order reactions. The model adopted for the calculations enabled high compliance and a good fit with the experimental data since it was able to capture both the degradation of the lignocellulosic fraction and the plastic fraction in the waste material. The authors recommend that researchers conduct TGA experiments on RDF samples to obtain a full picture of the material degradation process. If RDF was produced from household waste, the DTG degradation profile of this waste may match those reported in the literature. Nonetheless, if RDF was created from different waste streams and was heterogeneous, it is unlikely that a similar DTG profile would be found in the literature. By combining the obtained pyrolysis kinetics with heat and mass transfer, accurate simulation models for real thermochemical conversion systems can be obtained [147].

2.3. Tools for Numerical Simulation of Thermal Conversion Processes of Fuels and Waste

Among the most frequently mentioned programs for simulating thermal conversion processes, the literature on the subject mentions two commercial software programs: Aspen Plus and Fluent (version 2021 R2). It is emphasized that better simulation results can be obtained by using these programs simultaneously [1,148]. Few works, including those of the authors of the present article, mention Ansys Chemkin-Pro (version 2021R1) software as an irreplaceable tool for predicting the gaseous products of thermal conversion (Figure 10) [147,149].

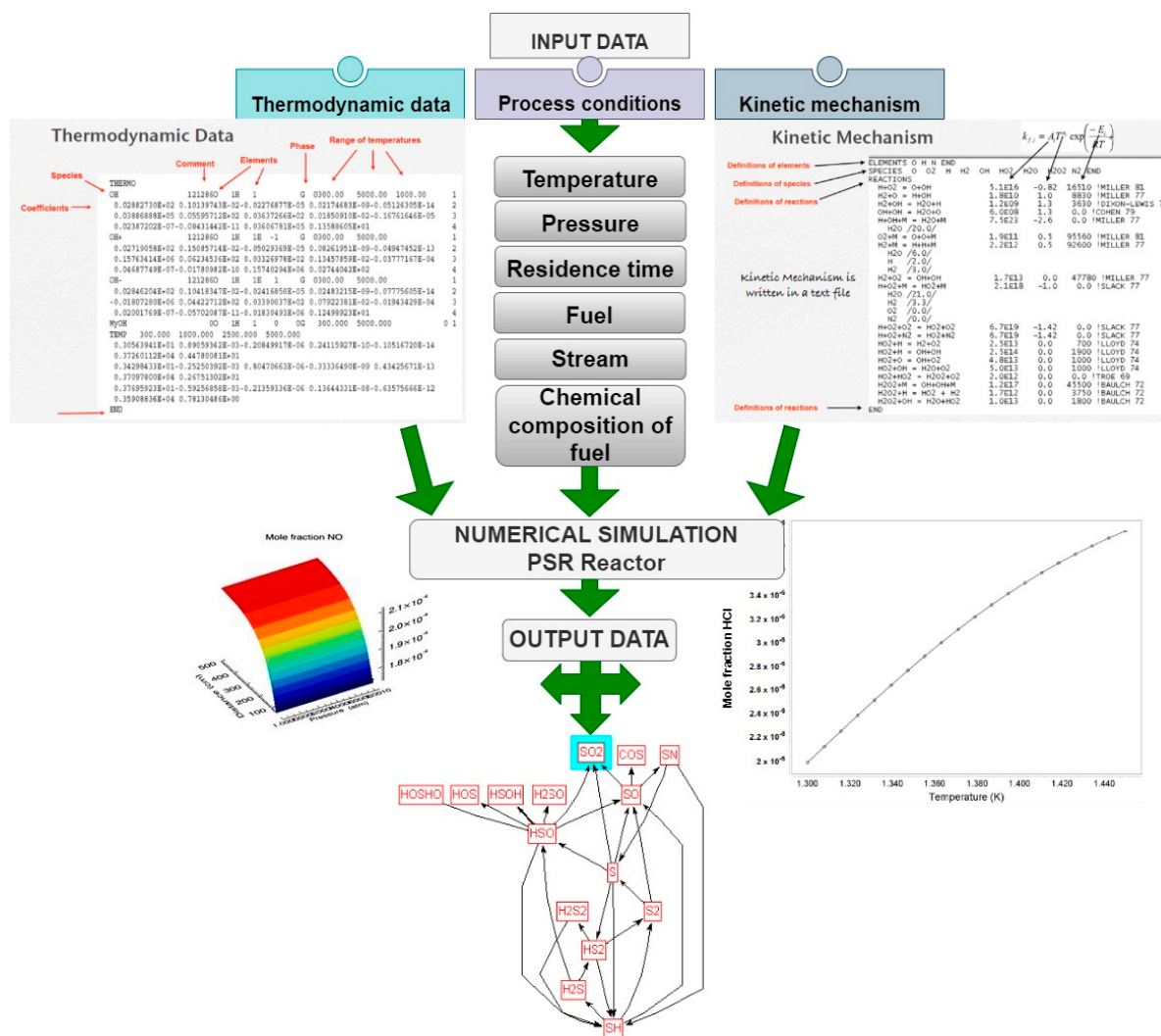


Figure 10. Diagram of procedure for modelling chemical composition of pyrolysis gas using Ansys Chemkin-Pro software [149].

To avoid the complexity of the thermal conversion process, e.g., gasification, and to facilitate the creation of models, some researchers have developed models based on the Aspen Plus process simulator. This involves assessing and analyzing each stage of the process, such as gasification, before integrating it into the global process [149–152]. Each stage of the process, e.g., gasification, can be described and tested in a block before it is integrated into the global process [153,154]. Simulation calculations using this tool are performed using the built-in database of the simulator's physical properties and the database of the properties of the chemical components used in the calculations (e.g., biomass). In addition, custom Fortran or Excel subroutines can be included if necessary [81]. The program uses a sequential modular approach to solve the process diagram module-by-module and calculate the outlet stream properties based on the inlet stream properties for each block. In

modelling, for example, a gasifier in Aspen Plus, the entire process is divided into several sub-processes, including drying and pyrolysis, oxidation and gasification or reduction.

In recent years, there has been a significant increase in the use of Aspen Plus models for thermal conversion processes, particularly gasification, compared to equilibrium models [150–152]. The literature review shows that most researchers rely on non-stoichiometric methods when modelling equilibrium using the Aspen Plus program. On the other hand, stoichiometric equilibrium models are rarely used in the literature, where only numerical models with fewer reactions are described. González-Vázquez et al. [81] compared a non-stoichiometric model and a stoichiometric model, both built using Aspen Plus, to determine their suitability for predicting steady-state biomass gasification efficiency. The simulation results were confirmed by experimental data previously obtained in a semi-pilot atmospheric pressure fluidized bed gasification unit. The authors used Aspen Plus V.8.6 to model biomass gasification and predict synthesis gas. The diagram presents each stage of the process, showing the flows of materials and energy are determined by means of operating blocks.

Models developed with the Ansys Chemkin-Pro tool, which enables accurate modelling of the thermal conversion reaction, e.g., biomass gasification, are definitely popular. The software offers users the ability to develop detailed reaction mechanisms and simulate the thermal decomposition of various raw materials, e.g., biomass, for various process conditions. Additionally, the tool can be integrated with computational fluid dynamics (CFD) models. According to the researchers, Chemkin-Pro is definitely more difficult to use than Aspen Plus, primarily as a consequence of the chemical approach to the analyzed process, based on chemical kinetics, which requires a deeper understanding of the chemical reactions and mechanisms, especially when describing complex biomass gasification processes. Additionally, the technical nature of the software makes it less user-friendly than Aspen Plus, which is designed for a wider range of chemical processes and has a more user-friendly interface. These factors make Chemkin-Pro require a higher level of expertise and effort to effectively utilize its chemical kinetic modelling capabilities in biomass gasification [99].

Examples of the use of Chemkin-Pro software are the simulations carried out by Sieradzka et al. [140] and Slefarski et al. [150]. The authors modelled the chemical composition of the gaseous products of the pyrolysis of fuels derived from waste and identified reaction paths based on kinetic models.

2.4. Validation Techniques of Chemical Kinetics Models in Waste Thermal Conversion Processes

To validate the results of the simulations of the thermal conversion processes of fuels and waste, experimental analyses are primarily used [151,152], including thermogravimetric analysis [111,153–155] with a Fourier transform infrared spectrometer (TG-FTIR) [156–158] and gas chromatography techniques [75,159–161]. Researchers may also compare their results with literature data [52,138].

One of the methods utilized to validate the results obtained by modelling is also statistical analysis employing statistical computing and software [162–164]: MATLAB, ANOVA (tool in OriginPro 2024b) version [165–168] and MS Excel (version 2021).

Statistical approaches [163–165,169], such as response surface methodology (RSM) and Taguchi, are commonly used to optimize experimental parameters (Figure 11). In the RSM optimization process, more series of experiments are usually performed than in the Taguchi method. The RSM model outperforms Taguchi in terms of precision and reliability, while Taguchi's approach is ideal for low-cost and rapid experimental studies. Researchers can choose between the RSM model and Taguchi's approach based on the complexity and financial resources required for their experiments. Several approaches to RSM have been developed over the years. Box Behnken design (BBD) and central composite design (CCD) technologies are the most commonly utilized RSM technologies for catalytic pyrolysis applications. Professor Taguchi developed optimization techniques (Taguchi techniques), which are commonly used to determine the optimal combination of parameters and their

impact on the objective function. Taguchi's optimization approach often uses the variance test, chi-square test and Fisher's exact test [170].

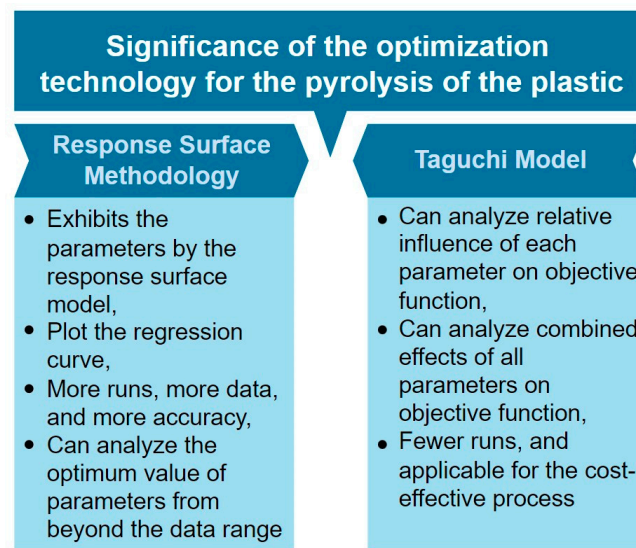


Figure 11. The comparison of response surface methodology and Taguchi method [170].

Regarding the Taguchi method and RSM, the literature has shown that both methods can provide satisfactory optimization results for selected applications, e.g., thermoelectric generators. However, RSM can provide a more comprehensive optimization analysis because it can show the influence of the parameters on the objective function and the interaction between the parameters. Moreover, in RSM, it is possible to visualize the results of the experimental analysis. The Taguchi method is unique in its ability to provide accurate optimization results with a small number of experiments, making it more cost-effective. The comparison and the most important steps of statistical optimization using the Taguchi, ANNOVA and RSM methods are presented in Figures 12 and 13 [165].

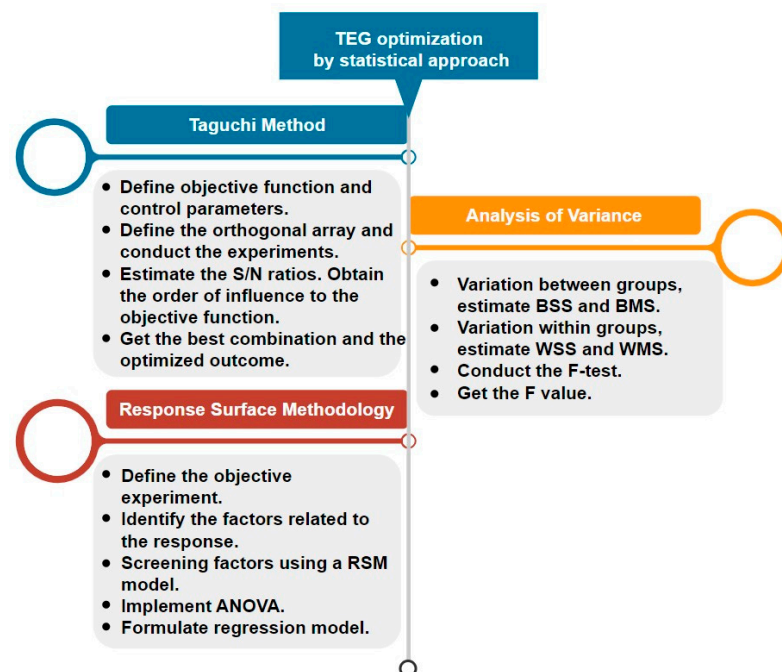


Figure 12. Comparison of optimization approaches for different methods [165].

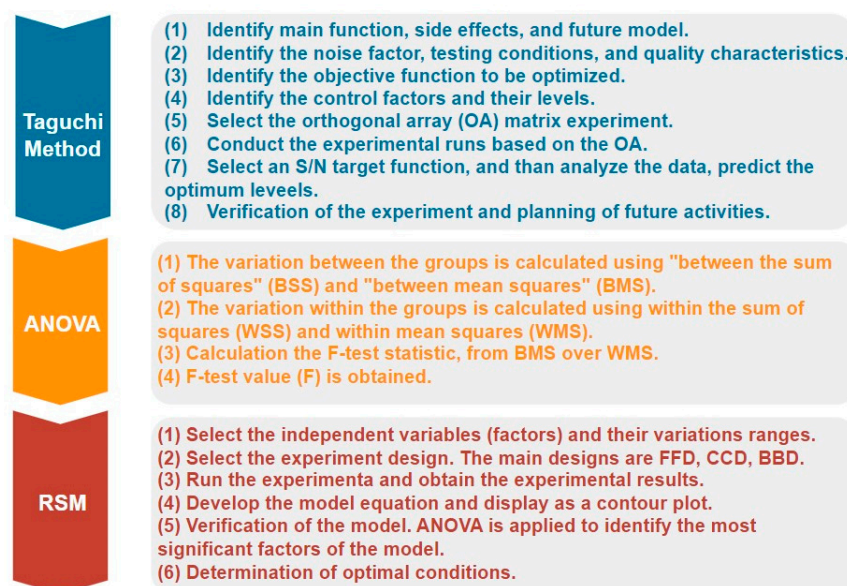


Figure 13. Steps of statistical optimization employing Taguchi, ANNOVA and RSM methods [165].

3. Results

As mentioned earlier, experimental analysis is one of the most frequently used methods to verify the obtained simulation results.

Peters et al. [138] compared the obtained simulation results, described in Section 2.2, with literature data, showing good agreement (Figure 14). Additionally, the authors conducted their pyrolysis experiments to validate the reaction model. The raw material used for the research came from beech wood and was subjected to pyrolysis under precisely defined conditions and at various temperatures. The result of the research was the determination of process efficiency in terms of the received products and their chemical composition. In the final stage, the composition of bio-oil obtained by simulating the pyrolysis of beech wood (moisture 8.9%) was compared with literature data, which showed that beech wood had a lower water content. Comparable proportions were found for organic acids and ketones, while much higher disproportions were obtained for alcohol and aldehyde. In the literature cited by the authors, as much as 44% of the bio-oil was not identified [138].

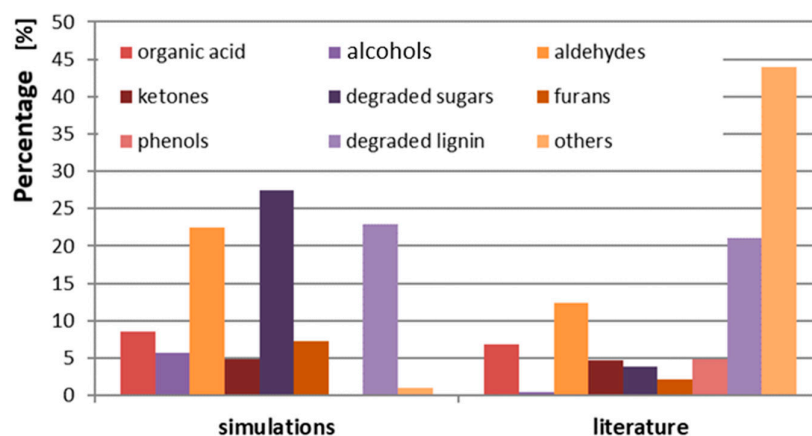


Figure 14. Comparison of the composition of bio-oil from beech wood pyrolysis obtained from simulation and literature data [138].

Ali et al. [171] conducted similar calculations using Aspen Plus software to model the chemical composition of the solid and liquid gasification products of a biomass and coal mixture, receiving results similar to those obtained in experimental studies (Figures 15–17).

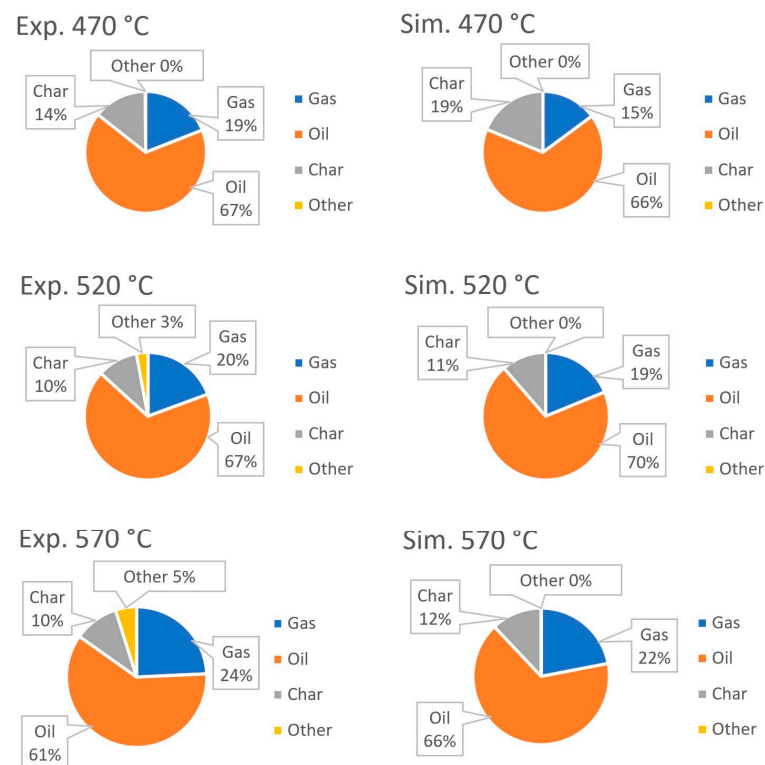


Figure 15. Fraction yield % [171].

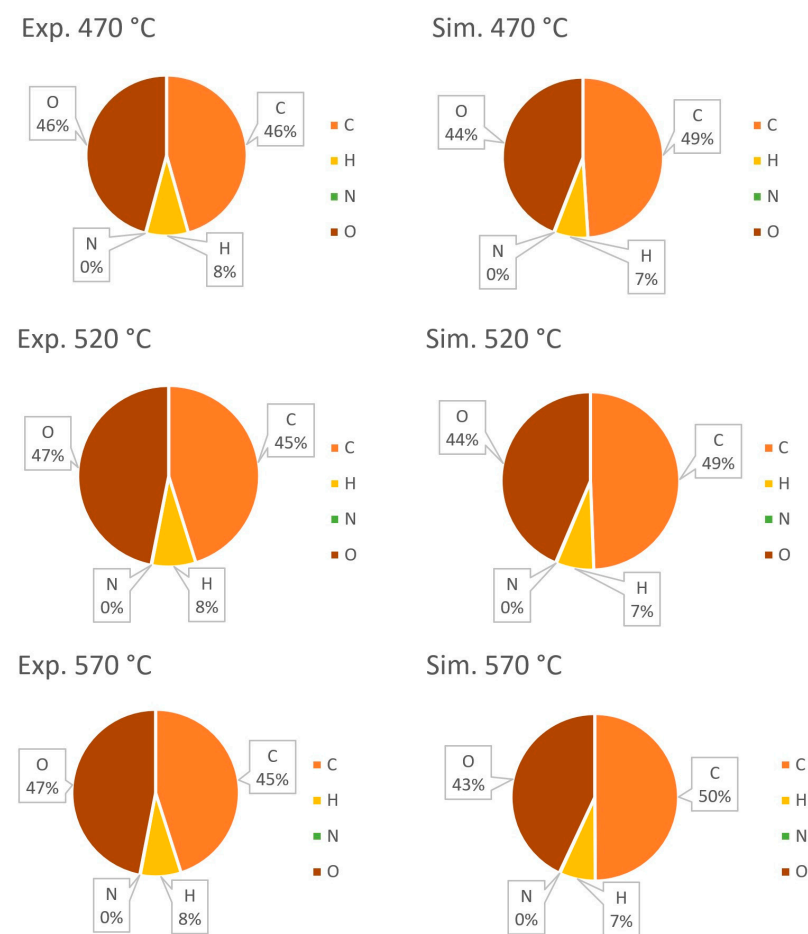


Figure 16. Bio-oil compounds [171].

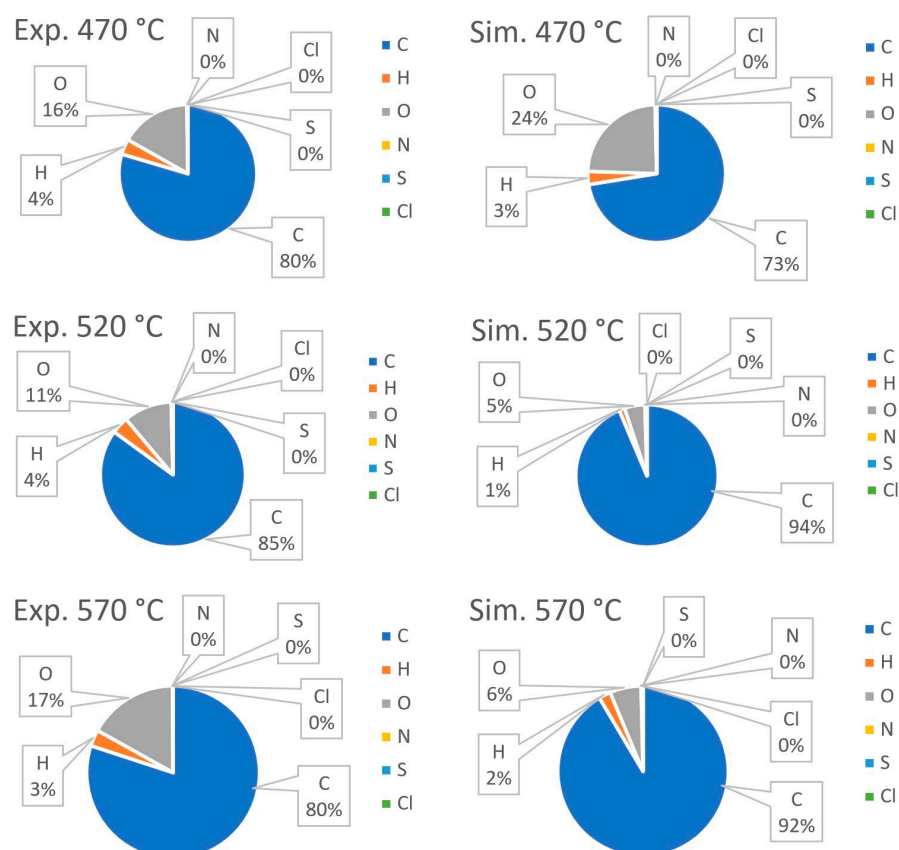


Figure 17. Char composition [171].

4. Discussion

In the era of energy transformation and decarbonization, many efforts are being made worldwide to promote the use of various types of waste as energy sources. These activities are aimed not only at searching for but also promoting sustainable alternatives, thanks to which waste will become a valuable raw material for other processes. Unfortunately, the heterogeneity and varied chemical composition of waste as well as the complexity of the phenomena occurring during thermal conversion make a comprehensive description of the degradation process difficult. This translates into limitations in their widespread use. Computer-simulation methods have been developed in recent years to address these issues, contributing to the intensification of research in the development of numerical models. The main efforts of many research centers around the world are primarily focused on understanding the gas dynamics and chemical mechanisms occurring during the thermal conversion of waste and, in particular, the reaction kinetics. The literature analysis carried out in this article shows that two commercial software products, Aspen Plus and Fluent, are most often used to simulate the processes of the thermal conversion of waste, while only a few works indicate Ansys Chemkin-Pro software as an irreplaceable tool for predicting the gaseous products of thermal conversion [147,149].

To summarize the topic discussed in this article, the following can be noted:

1. The analysis carried out with the use of the VOSviewer software shows that, despite many scientific works published on this topic, there is still a research gap in the issues discussed in the article.
2. The literature on the subject emphasizes that a number of factors are responsible for the proper use of computer simulation methods, and the most important advantage is the ability to simulate phenomena that are difficult or impossible to implement in real conditions.

3. The results of numerical modeling using simplified chemical mechanisms (CFD modeling) describing the combustion process are subject to large errors (due to the long calculation time, simplifications of chemical kinetics are used in the computational procedure, namely reducing the chemistry of methane oxidation to a single-stage mechanism in which combustion products are CO_2 , H_2O , O_2 and N_2), which is why they often do not coincide with actual measurements. The assumption of a simple combustion mechanism in the calculations results in significant discrepancies with the measurement results.
4. Due to the possibility to create a multi-stage, complex model in the ANSYS Chemkin-Pro program, which does not use simplifications in thermodynamics and chemical kinetics, various waste thermal processing processes can be modeled with high accuracy.
5. The cost of building a model is often much lower than conducting experimental research, resulting in significant savings in time and money.
6. Computer simulations also have several disadvantages, the most important of which is the possibility of making an error when creating a model that omits parameters and chemical reactions that are important from the point of view of the analyzed process.
7. Moreover, numerous works indicate difficulties and errors when interpreting the obtained simulation results. The above-mentioned defects are the responsibility of humans, who may not only incorrectly formulate the simulated problem and adjust the tool but may also draw incorrect conclusions from the performed simulations.
8. It is crucial to validate the developed model and verify the obtained calculations through experimental means using statistical analysis (e.g., MATLAB, ANOVA) or based on literature data. Without such validation, the results of the model calculations remain hypothetical.
9. The issue of managing environmentally burdensome gaseous products of thermal conversion of calorific waste is of an applied nature, as evidenced by the interest of both entrepreneurs from the waste and metallurgical industries. However, this direction requires extensive theoretical studies in the analysis of chemical mechanisms.
10. Knowledge of chemical mechanisms describing the process of combustion or co-combustion of gases from the thermal conversion of waste will create the possibility of their energy utilization.
11. Providing comprehensive knowledge about combustion kinetics will also enable taking appropriate actions to manage gases after thermal conversion of waste while maintaining the proper operation of the heating chamber and minimizing pollution.
12. Currently, it is particularly important and problematic to properly identify the chemical composition of exhaust gases while, at the same time, focusing on activities aimed at minimizing harmful pollutants, such as PAHs.

The analysis conducted in this article indicates enormous progress in modelling the processes of the thermal conversion of waste. This suggests that numerical simulations will likely replace costly experimental research in the future. Nonetheless, it is important to consider that, as the number of phenomena to be modelled increases, the accuracy of the model also increases, resulting in a better reflection of reality, but, at the same time, requiring a longer calculation time and greater computing power, leading to higher costs. Moreover, thermal management of waste towards the recovery of valuable products, such as pyrolysis gas, biochar and condensate, as is the case in the pyrolysis process, is an additional opportunity to improve energy efficiency. Using the potential of post-process gases, especially gases from the pyrolysis process, e.g., of biomass, will have an economic impact, contributing to lower fuel consumption.

5. Conclusions

To sum up, it is important to note that, despite the disadvantages and difficulties associated with creating advanced simulation projects, they are an integral element of the development of all industries. The use of simulation in thermal waste conversion processes is an opportunity to employ them on a wider scale, thanks to a better understanding

of the phenomena occurring during their degradation, both gasodynamic and kinetic. The analysis performed using the VOSviewer software indicates the need to develop mathematical models used when modeling thermal processes. Reducing the expenditure that would be necessary for extensive experimental research will contribute to a faster transformation of a linear economy into a circular economy that promotes the efficient use of waste.

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