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Modeling and simulation of a fixed bed gasification process for thermal treatment of municipal solid waste and agricultural residues

Matheus Oliveira[a], Ana Ramos[b], Eliseu Monteiro[c], Abel Rouboa[b,d,*]

[a] ECT/UTAD, School of Science and Technology, University of Trás-os-Montes e Alto Douro, Vila Real, Portugal
[b] LAETA-INEGI, Institute of Science and Innovation in Mechanical and Industrial Engineering, 4200-465 Porto, Portugal
[c] LAETA-FCTUC, Faculty of Sciences and Technology of the University of Coimbra, R. Sílvio Lima, 3030-790 Coimbra, Portugal
[d] MEAM - School of Engineering and Applied Sciences, University of Pennsylvania, PA 19104-6391, USA

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Abstract

This work aims to develop a numerical simulation model of the combined and integrated production process of combustion and gasification, for a synthesis gas production system (SYNGAS), fed with municipal solid waste (MSW), agricultural and forestry waste. For this purpose, the EMSO software (Environment for Modeling, Simulation, and Optimization) was used in the formulation of a fixed-bed gasifier with the co-current flow. The model is developed based on mathematical calculations of partial differential equations, being one-dimensional (1-D), and considers chemical kinetics, diffusivity, and heat and mass transfer phenomena. Its validation is based on data available in the literature (variables, initial and operational conditions). As a result, a simulation of a gasifier was obtained, capable of predicting the production of Syngas, having a good correlation with the published experimental results. The general data obtained were in agreement, with high consistency for the analysis of the pilot plant in the laboratory and semi-industrial scale for solid waste processing. However, detailing the behavior of the gasifier is essential to maximize the efficiency of the process. For that, the numerical simulation tested several operational parameters, such as air–fuel ratio and gasifier temperature for instance.

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Keywords: Gasification; Syngas; Solid residues; Circular economy; Modeling; Fixed bed

1. Introduction

Waste management should increasingly be a priority in adopting public policies, whereas a more efficient management of natural resources and the consequent reduction of associated environmental impacts would create business opportunities, also promoting new jobs [1,2]. The European Commission and other regulatory bodies enforce circular economy as a tool to increase sustainability, having set challenging ambitions such as achieving carbon neutrality, promoting an efficient use of resources, and keeping them in the economy at their highest value for

* Corresponding author at: MEAM - School of Engineering and Applied Sciences, University of Pennsylvania, PA 19104-6391, USA.
E-mail address: rouboa@utad.pt (A. Rouboa).

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longer [3–5]. Population increase is directly related to the generation of municipal solid waste (MSW). Therefore, under the circular economy view, it is essential to reintegrate waste into the value chain, reducing the impacts caused to the environment, guaranteeing human and animal health [6]. Currently, the most common methods of solid waste disposal are landfills and incineration. However, there are more adequate techniques to deal with this problem, such as gasification, the conversion of waste into energy, and synthesis gas generation. In other words, this operational application would have the dual benefit of reducing the amount of waste deposited in landfills while recovering its heat, which may be used to produce electricity. This synthetic gas can, subsequently, be converted into electrical energy, playing a vital role to meet the future global energy demand [7–9]. In comparison to other techniques (such as combustion and pyrolysis), gasification requires lower temperatures and produces less pollutants. Still, the worldwide gasification of solid waste is not used to its full capacity [10].

Gasification is defined as a method in which the raw material molecules are broken down into their elements at high temperatures (between 500 and 1400 °C) and atmospheric or elevated pressures (up to 33 bar) [11]. Gasifying agents such as steam, air, O_2, CO_2 or mixtures thereof can be utilized in the process [12–18]. Exposure of the raw material to the sub-stoichiometric level of oxygen leads to the production of synthetic gas mainly composed of hydrogen, carbon monoxide, methane, carbon dioxide, branched hydrocarbons, tar and a negligible amount of nitrogen [19]. This gas has applications such as combustion in engines for the production of electric energy, heat generation, raw material in chemical synthesis, among others [15], in similar systems to the one presented in Fig. 1. Tar, which can be categorized as primary, secondary alkyl, tertiary and condensed tertiary, is a dark viscous liquid consisting mainly of aromatic hydrocarbons from a single ring to benzene units also formed in the process [20].

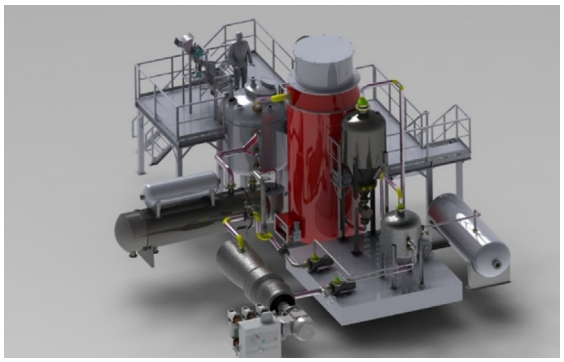

Fig. 1. 3D modeling of the waste processing plant.

Pyrolysis is the first step of gasification. Here, the high temperature destroys a combination of organic molecules, causing the organic compounds contained in the residues to detach and volatilize. When steam enters the processing chamber, these components are converted into synthesis gas. Then this gas is cleaned, a mixture of CO, CO_2 and H_2 being achieved by the steam reforming reaction. Other residual components that do not volatilize are transformed into a molten state and then cooled to form a glassy state, in the case of plasma gasification. The vitrified residue, has a chemical stability providing environmental benefits, as it has high resistance to the leaching of dangerous components, which adhere to glass, and has interesting downstream applications [17].

Syngas is mainly composed of carbon monoxide and hydrogen (CO and H_2, respectively). Currently, the use of gasifiers is not only restricted to use in the chemical and petrochemical industries but also has a wide range of applications in many other fields (industrial and domestic). According to Gómez [21], there are four basic reasons to gasify biomass for energy purposes: (1) it is a natural and renewable resource, with high availability and relative ease of use; (2) it represents a renewable and safe source of energy that is not adjusted to changes in prices and supply in the foreign market; (3) its use allows developing countries to decrease their external dependence on oil; (4) from an energy point of view, it is a clean fuel when compared to fossils. All energy sources have limitations, nevertheless biomass is a relatively low-cost and clean energy source, but its production is limited, above all, by economic factors [10,22,23]. In addition, it is noteworthy that biomass gasification can be considered a carbon-neutral technique [24,25], legally complying with pollutant emissions [16,26], and accounting for high compaction rates through gasification, that is, reduction of mass and volume of solid waste [27].

A gasifier is a very complex system, not only due to the operational conditions but also to the chemical reactions entailed [8], therefore the use of efficient numerical models is highly necessary, to predict the final output as well as optimize the system design [7]. Mathematical computational models can provide quick and accurate insights, by simulating a variety of experimental conditions (temperature, vapor/biomass ratio, catalyst type, mixture composition, among others) before applying them in the real facilities. Therefore, sensitivity analysis and parametric optimization might be readily performed, leading to considerable savings in time and resources. Computational fluid dynamics (CFD) is one of the preferred numerical approaches for gasification systems [22,23,28–30]. Municipal waste and forest/agricultural residues have been massively studied, different operational parameters being reported in the most diverse references [9,18,24–26]. CFD enables the development of mathematical models such as kinetic and thermodynamic equilibrium models [16,17,22,23,29,31].

IGCC (Integrated Gasification Combined Cycle) is a Rankine cycle process that combines the production and purification of syngas with its use in a turbine to produce clean, affordable energy. The integration of this energy conversion process allows the use of resources and energy generation with high efficiency and very low levels of pollution. In addition, the IGCC system is quite flexible in terms of raw materials, as it can convert almost any type of carbon-based feedstock into useful chemicals and energy [32]. The first step of the IGCC is partial oxidation using a gasifier, where residual moisture is removed from the raw material. In the second stage, the gasification stage, the conversion of solid and liquid waste into gaseous products takes place, eliminating the volatiles, which may be used in gas turbines. The turbine combustor is utilized to completely oxidize the previously produced gas, after purification to remove particles (sulfur compounds and nitrogen oxides).

This work aims at modeling the gasification reactor, developing a one-dimensional model to simulate the gasification of agro-industrial waste in a fixed bed. The numerical results obtained were validated according to an experimental dataset of a semi-industrial fixed bed gasifier [10,33]. Simulation of operating parameters can predict the effect of moisture content, air–fuel ratio and gasifier temperature, among others. This model proved to be very effective in predicting a different set of responses for each situation, considering that the model can be used for different raw materials, such as MSW, agricultural and forestry residues or mixtures.

2. Model description

The combined gasification and combustion technology for the thermal treatment of waste, seen in Fig. 1, was simulated using a computational model. Therefore, the description in the next sections relates to this system.

In this study, the operational parameters simulated by the model considered only the steady-state and the primary airflow (102.4 Nm^3/h). This flux corresponds to $\varphi = 0.33$ considering the oxygen consumption for the complete combustion of biomass equal to 1.57 kgO_2/kg_B, as seen in [10,34,35]. The reactor core is a conventional fixed bed downstream gasification reactor. The reactor is a fixed-bed gas cylinder with a kinetic (1-D) model developed for the fusion and gasification process. For kinetic modeling, the reactor is divided into four sections and the process of each section is studied separately (Fig. 2).

The dimensions adapted for simulating the gasifier were the same used in [10], cross-sectional area of 1.95 m and height of 0.63 m^2. However, they can undergo changes and evaluations as to the possible effects in determining the residue drying zone, the loss of volatile substances, the injection of gasification agent and the generation of fuel gas. These processes characterize the four theoretical zones in the reactor from top to bottom: (1) drying zone (> 150 °C), (2) pyrolysis zone (150–700 °C), (3) oxidation zone (700–1500 °C) and (4) reduction zone (800–1100 °C). These four areas are the classic and idealized phases reported in literature [34].

In the drying zone, the residual moisture that enters the reactor decreases, due to the contact with the hot exhaust gas at the top of the reactor, drying the feedstock. According to [36], the evaporation temperature at the pressure of atmospheric residual moisture is assumed to be 120 °C. The behavior of the temperature gradient in the gasifier was modeled taking into account the losses to the medium and the energy needed to perform the heating seen in Fig. 3.

In the pyrolysis zone (Fig. 2), the process is then carried out using a set of mass balance equations, removing the moisture in the dry MSW feed used in this simulation. Before starting the pyrolysis process, the MSW must be considered as being just a solid, excluding the effects of liquefaction. The biomass pyrolysis process starts at 200 °C and ends at 500 °C. When increasing the temperature to more than 500 °C, the primary tar changes becoming gas and secondary tar.

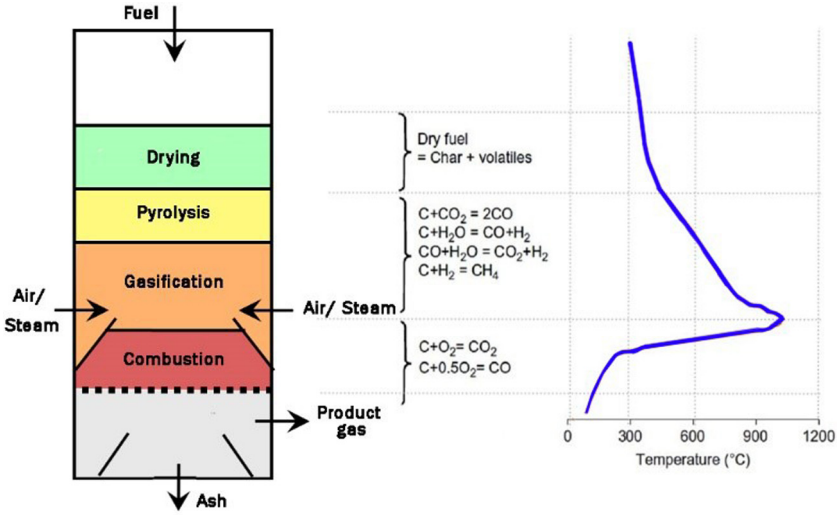

Fig. 2. Process diagram and temperature variation.
Source: Adapted from [20].

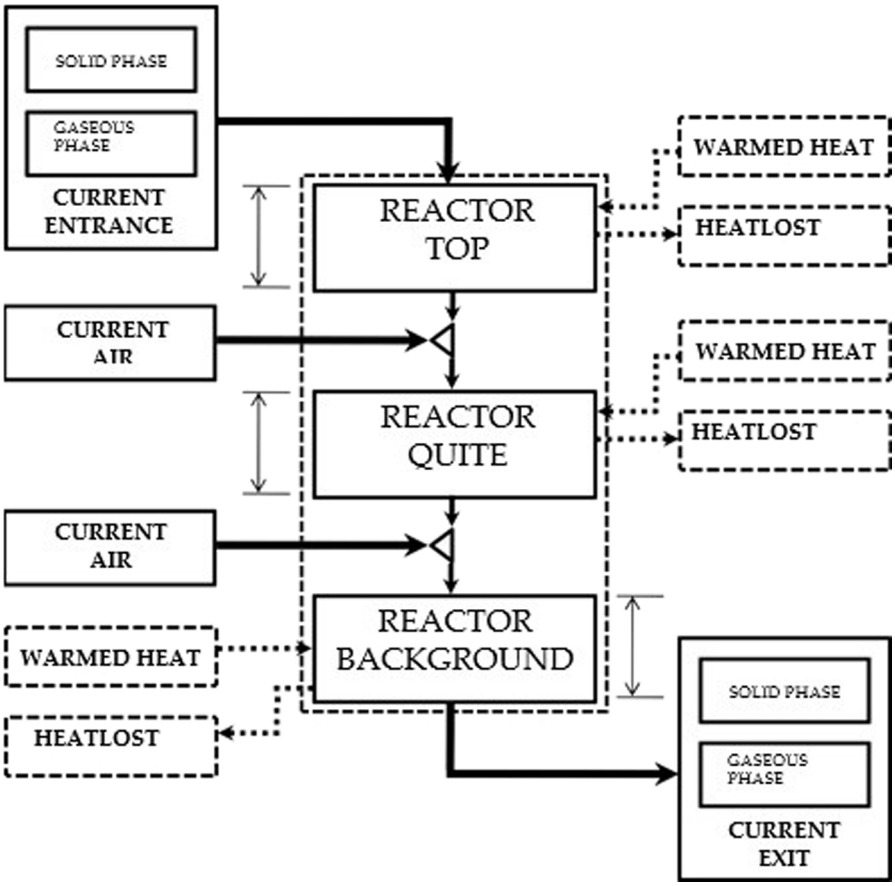

Fig. 3. Schematic diagram of the model at EMSO [18].

Finally, in the gasification step, thermal decomposition happens, producing gaseous agents (H_2O and O_2). Depending on the profile of the studied sample and operating temperature inside the gasifier, the reactor is divided into two regions: high temperature (HTZ) and low temperature (LTR), which vary according to a temperature gradient. As a result, the organic gasification process of the MSW is carried out operating at a temperature of about 800 °C–1200 °C, the gasification process is complete, and the organic portion is converted into syngas.

2.1. Thermodynamics

Numerical gasification simulations include the calculation of continuity, heat transport and diffusivity equations. In the current model, complex phenomena, such as chemical reactions, must be simulated in a simplified way, disregarding the gas–solid coupled flow that is difficult to implement, such as in turbulent conditions. The initial stage of the gasification process starts with the decomposition region (pyrolysis) and continues with the combustion region, seen in Fig. 2. The relevant reactions considered in these processes are shown in Table 1 [37]:

Table 1. Chemical reactions involved in gasification process [10,37].

Reaction	Chemical reaction	Process
	Solid phase	
m	$H_2O_{(l)} \xrightarrow{k_m} H_2O_{(g)}$	Evaporation
(p_1)[a]	$B \xrightarrow{k_{p_1}} 0,7389C + 0,1182CO + 0,2266CO_2 + 0,0345H_2 + 0,0788CH_4 + 0,4581H_2O + 0,03941T$	Primary pyrolysis
(p_2)[a]	$T \xrightarrow{k_{p_2}} 0,3663CO + 0,4488CO_2 + 0,1848CH_4$	Secondary pyrolysis
	Gaseous phase	
(c1)[a]	$CH_{0,7393}O_{1,264} + 0,0528O_2 \xrightarrow{k_{c_1}} CO + 0,3696H_2O$	Tar combustion
c2	$CH_4 + 1,5O_2 \xrightarrow{k_{c_2}} CO + 2H_2O$	Methane combustion
c3	$2CO + O_2 \xrightarrow{k_{c_3}} 2CO_2$	Combustion of carbon monoxide
c4	$2H_2 + O_2 \xrightarrow{k_{c_4}} 2H_2O$	Hydrogen combustion
wg	$CO + H_2O \xrightarrow{k_{wg}} CO_2 + H_2$	Water–gas shift reaction
	Heterogeneous reactions	
g1	$C + CO_2 \xrightarrow{k_{g_1}} 2CO$	Boudouard reaction
g2	$C + 2H_2 \xrightarrow{k_{g_2}} CH_2$	Methanation reaction
g3	$C + H_2O \xrightarrow{k_{g_3}} CO + H_2$	Water vapor gasification
c5	$C + O_2 \xrightarrow{k_{g_5}} CO_2$	Combustion of carbonaceous material

[a]Calculated from Font et al. [38] e Di Blasi (2000) [39].

The mass balance for the system can be represented by global balance expressions and components with terms advective, accumulation, diffusive and generation. According to [10], 11 chemical species are considered, of these 3 solid components: biomass (B), moisture (M) and residual carbon (C), and 8 gaseous: tar (T), water vapor (H_2O), oxygen (O_2), nitrogen (N_2), carbon monoxide and dioxide (CO and CO_2, respectively), hydrogen (H_2) and methane (CH_4). The equations and reactions followed are (1)–(29).

Balance for the solid phase

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial(\rho_i U_s)}{\partial z} = \sum_{j=1}^{N_{rs}} \upsilon_{i,j} R_j \tag{1}$$

where N is the total number of species, υ_i the number of moles of the species, and R_i the chemical potential of the species i. Given $i = B, M, C$ and $j = m, p_1$

With except N_2, the balance for the gas phase:

$$\varepsilon \frac{\partial \rho_i}{\partial t} + \frac{\partial(\rho_i U_s)}{\partial z} = \frac{\partial}{\partial z}\left(D\rho_g \frac{\partial x_i}{\partial z}\right) + M\omega_i \sum_{j=1}^{N_{rs}} \upsilon_{i,j} R_j + \omega_i \tag{2}$$

In which $i = T$, O_2, CO_2, H_2, H_2O, CH_4, CO and $j = m$, c_1–c_5, g_1–g_3, ω_g. The term ω_i represents the number of gaseous species i produced by a chemical reaction in the solid phase, represented in Table 1. It must be obtained from the following formula [40,41];

$$\omega_i =_i \sum_{j=1}^{N_{rs}} v_{i,j} R_j \tag{3}$$

Where $i = B, M, C$ e $j = p_1, p_2$.

The mass concentration of nitrogen (N_2) is calculated by difference of the total quantity ρ_g, mass concentration of the gas phase:

$$\rho_{N_2} = \rho_g - \sum_{i \neq N_2} \rho_i \tag{4}$$

In which ρ_g is given by the law of ideal gases:

$$PM\omega_g = \rho_g R T_g \tag{5}$$

Overall balance for the solid phase:

$$\rho_s \frac{\delta U_s}{\delta z} = \sum_{i=1}^{N_{cs}} \sum_{j=1}^{N_{rs}} v_{i,j} R_j \tag{6}$$

Continuity equation:

$$\varepsilon \frac{\partial \rho_g}{\partial t} + \frac{\partial(\rho_g U_g)}{\partial z} = \sum_{i=1}^{N_{cs}} \sum_{j=1}^{N_{rs}} v_{i,j} M \omega_i R_j + (1 - vc,_{p1}) R_{p1} + \sum_{i=1}^{N_{cg}} v_{i,p2} R_{p2} \tag{7}$$

Where $i = T$, O_2, CO_2, H_2, H_2O, CH_4, CO, N_2e $j = m$, c_5, g_1–g_3, ω_g. The terms on the right side represent the production rates of all gaseous species.

Energy balance

Energy balances consist of the terms of accumulation, heat by conduction and advection, heat from chemical reactions, and heat exchanged between the phases and the wall, as shown below:

Energy balance for the solid phase:

$$\frac{\partial(\rho_s H_s)}{\partial t} = \frac{\partial}{\partial z}\left(\lambda_s^* \frac{\partial T_s}{\partial z}\right) + \frac{\partial(U_s \rho_s H_s)}{\partial z} - \sum_{j=1}^{N_{rs}} R_j \Delta H_j - Q_{sg} - Q_{s\omega} \tag{8}$$

Where $i = B, M, C$ e $j = c_5$, g_1-g_3, p_1, m.

Energy balance for the gaseous phase

$$\varepsilon \frac{\partial(\rho_g H_g)}{\partial t} = \frac{\partial}{\partial z}\left(\lambda_g^* \frac{\partial T_g}{\partial z}\right) + \frac{\partial(U_g \rho_g H_g)}{\partial z} - \sum_{j=1}^{N_{rs}} R_j \Delta H_j - Q_{sg} - Q_{s\omega} \tag{9}$$

Where $i = T$, O_2, CO_2, H_2, H_2O, CH_4, CO, N_2 e $j = c_1$–c_4, ω_g, p_2.

The heat exchanged between the solid and gaseous (Q_{sg}) phases and the heat exchanged from the wall to the solid (Q_{sw}) and gaseous (Q_{gw}) phases are given by:

$$Q_{sg} = h_{sg} \upsilon_p (T_s - T_g) \tag{10}$$

$$Q_{sw} = \frac{4h_{sw}}{d_r}(T_s - T_w) \tag{11}$$

$$Q_{gw} = \frac{4h_{gw}}{d_r}(T_g - T_w) \tag{12}$$

Reaction rates

Drying:

$$r_1 = \left(1 - \alpha_g\right) A_1 exp\left(\frac{-E_1}{RT_s}\right) \rho_m \tag{13}$$

To assign the values of the equated parameters, data from references [42–48] were used. Throughout a chemical combustion reaction, a wide variety of intermediate reactions occur, due to the influence of several factors, including the diffusion of reagents, the breaking of the binding of solid compounds, as well as the interactions between the streams and the flow regime. For this reason, several previous models have been combined into a single Kinetic/Diffusion Surface Reaction Model to represent the effects of free radical polymerization [17,22,23,28,30,49,50].

$$R_c = \frac{P_{O_2}}{\frac{1}{K_r} + \frac{1}{K_d}} \tag{14}$$

$$K_d = \frac{5.06 \times 10^{-7}}{d_p} \times \left(\frac{T_s + T_g}{2}\right)^{0.75} \tag{15}$$

$$K_r = A_c T_s exp\left[\frac{E_c}{RT_s}\right] \tag{16}$$

2.2. Model assumptions

In developing the proposed model, the kinetics of the main reactions involved and the phenomena of heat and mass transfer between solid and gaseous compounds and the walls of the gasifier are considered. The developed model is based on the stationary model proposed by [47]. They simulate the mass and energy conservation equations, so that the terms generators, consumers and accumulators are described by the physical relationships (heat and mass transfer) and chemical (kinetics).

Model input parameters are: reactor dimensions, operating conditions, phase inlet temperatures, pressure, concentrations, flows, and reactor wall temperature. Some of the estimated variables are: gradient temperature, pressure, the concentration of species and phase flows.

The following restrictions were adopted in the model:

- Behavior of the gas phase as an ideal gas.
- Co-current flow only with the solid and gas phases involved;
- Dynamic and one-dimensional system (1-D model);
- Ballast wall as sole source/heat sink;

From the co-current flow of the solid and gaseous phases along the reactor bed, the following processes are considered:

1. Drying of biomass;
2. Devolatilization of biomass and thermal degradation of tar;
3. Carbonaceous material combusts and gasifies;
4. Combustion of volatilized species;
5. Resistance to extra-particle mass transfer;
6. Transfer of mass through the bed between the solid and gaseous (moisture) phases;
7. The reactor wall and the phases transfer heat to each other;
8. Heat transfer by radiation;
9. Absence of thermal equilibrium between the solid and gaseous phases;
10. Variable flows of the solid and gaseous phases

2.3. EMSO modeling

The model diagram created in EMSO can be seen in Fig. 3. Waste enters the system through the waste stream. The simulator EMSO (Environment for Modeling, Simulation and Optimization), introduced by Soares and Secchi [33], has characteristics that set it apart from other free simulators, and even from most commercial packages. It is an equation-driven type and allows the user to freely create and modify models through its own modeling language, which is intuitive and easy to use, based on two basic entities called Model and FlowSheet. The first is suitable for describing individual models, as for each piece of equipment; the second, on the other hand, is suitable for

describing systems, flowcharts, composed of models and their connections. The software also offers the possibility to define models as subtypes of other models through an inheritance concept.

Thus, the aim of this work is to develop a library of mathematical models for simulating processes involving particulate solids through the EMSO simulator, which does not have native models for such systems.

An extensive bibliographic search on the characteristics of particulate systems and their unitary operations was carried out, contemplating purely solid and solid–fluid systems. The model was implemented in the EMSO simulator in a structured way, using the object-oriented language. Gas flow, solid flow, air flow and kinetic model were described in different entities and sub-entities, using the concepts of composition and inheritance (Fig. 3).

The entity "input current" is internally composed of the initial currents: solid phase and gas phase. The main kinetic model is a single entity, but it is divided into "reactor top", "reactor quite" and " reactor background" according to the height of the gas flow inlet, as shown in Fig. 3. The calculation routines of the kinetic model return output data are then passed on to the next step plus an air current. "Lost heat" represents the heat lost by the walls to the external environment. This application example, with 50 points of discretization, results in a problem of 16,426 variables, 16,399 equations and 27 specifications, conform to what was suggested by [10].

3. Materials and methods

3.1. Fuel

The waste used as fuel in this study is a combination of solid urban waste and forestry waste. In most cases, they are a mixture of these forms with different amounts of chemical species. According to the literature [51], the profile of the studied sample is shown in Table 2. Therefore, this global chemical composition will be considered in the next sections to perform a sensitivity analysis of this compound. Solid waste does not exist in the EMSO software database, creating a challenge to define this material in the software. The method used in this model is based on the complete decomposition of the residues or the complete pyrolysis of the residues.

3.2. Model validation

According to the bibliographic review, the residues are predominantly plastic (50.54% by mass), in addition to paper (7.54%), fabric (9.95%), rubber (5.55%) and garbage in general [44]. For the operation of the pilot plant, only the processed waste was considered. This simulation is developed under the assumption that the residence time is long enough to allow the chemical reactions to reach an equilibrium state. The characteristics of MSW and input parameters of gasifier operating conditions are given in Table 2. Ashes were also defined as a non-conventional component with an ash content set to 100%.

Table 2. Municipal solid waste characterization [10,51].

Ultimate analysis (%)		Proximate analysis (%)	
C	47.9	Volatiles	77.6
H	6.0	Fixed carbon	10.7
O	32.9	Moisture	20
N	< 1.2	Ash	11.7
S	0.3	LHV (MJ/kg)	12.890

3.3. Gasifier

The fixed bed combustion reactor with co-current flow used experimentally, has as main characteristics: a total volume of 0.730 m^3, receiving four air injections for oxidizing the fuel gas generated, due to the reactor operation specification in co-current with air injections at 81 cm and 15 cm above the grid (reactor bottom). According to the injections of oxidizing agent, the reactor chamber was divided into 4 zones: primary combustion zone, secondary combustion zone, tertiary combustion zone and quaternary combustion zone [34].

The load fed in semi-batch is received in the supply chamber with a volume of 0.25 m^3, being hermetically closed by means of an external and an internal cover.

The primary combustion zone, with a total volume of 0.160 m^3, is located below the grate, right at the end of the reactor. In this chamber there is an expansion and the start of combustion of the fuel gas coming from the reduction zone of the gasification stage. Below this zone is located the ashtray, with a total volume of 0.110 m^3, where the ash with a larger particle size is collected.

Secondary air, preheated by passing through the grate, is injected through ducts distributed in the initial section of the secondary combustion zone, with a total volume of 0.042 m^3. In this zone, there is an increase in the turbulence of the gases coming from the gasification reactor, with a view to increasing the efficiency of combustion.

The tertiary combustion zone has a cylindrical shape with a total volume of 0.458 m^3, being lined with refractory material and designed to ensure the complete combustion of the combustible gases formed. It has an afterburner that is used to start the equipment. The exhaust of flue gases takes place horizontally in the center of this zone. Finally, there is the final combustion step taking place in the quaternary combustion zone. This zone has a cylindrical shape with a total volume of 0.075 m^3 and is located downstream of the previous tertiary combustion zone.

4. Analysis of results

For the process of gasification on a laboratory or semi-industrial scale for MSW, in a fixed bed gasifier reported by [10], a simulation of a downdraft fixed bed biomass gasifier is proposed. It is noteworthy that one of the main advantages of the model developed here is the inclusion of tar in the kinetics of the reactions involved, seen in Table 2, represented by the p2 T (tar) reaction, as this can drastically increase the precision of the proposed model.

4.1. Numerical model validation

In this section, the validation of the model is shown, which can be endorsed with the data and experimental results provided by [10,34,35,47,52]. The deviation of results was quantified using relative error. The results for the validation of the model may be seen in Fig. 4, the concentration of syngas components being shown.

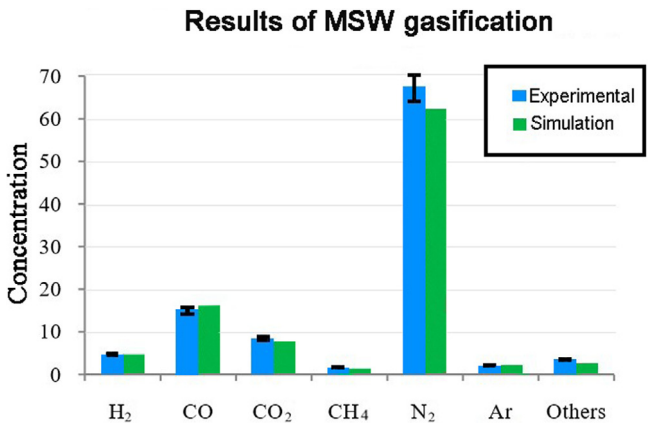

Fig. 4. A comparison between experimental and simulation results of syngas composition.

Fig. 4 shows that the simulation results are consistent within the 96% confidence level, mainly in terms of the methane reaction. The percentage of relative error obtained for the main gaseous components of the synthesis gas is 8.2% for N_2, 2.15% for H_2, 14.1% for CO_2, 8.9% for CO and 3,77% for CH_4. In a study conducted by [53], the excessive prediction of the H_2 content compared to the experimental results is closely related to the negligence of tar formation in all phases of gasification. A major problem with tar modeling is the chemical uncertainties of tar compositions, many models developed related to biomass gasification ignore tar modeling due to its complexity, which is not neglected in this proposed model, considering the influence of this variable in the modeling. Tar is predominantly determined by the operating condition of the gasifier. Despite variations in the chemical compositions of the tar produced, in different studies it was included in the modeling in different ways. [54] considered tar as a mixture of benzene, toluene and naphthalene. During an investigation conducted by [55] and [56], tar was modeled as phenol and toluene, respectively. It is important to emphasize that, regardless of the chemical composition of the

tar, its inclusion in the model as a modification strategy can improve the model's credibility. [57] explain that the inclusion of tar in the mass balance equation brings a notable increase in model accuracy.

Once validated, the model was utilized to analyze the influence of some parameters and variables, such as air–fuel ratio and gasification temperature, as seen in Sections 4.2 and 4.3.

4.2. Equivalence ratio effect

For energy generation, the combination of hydrogen and methane in the synthesis of gas is of great relevance. To investigate the amount of methane, several parameters such as the Equivalence Ratio (ER), which is an important parameter in the analysis of a gasifier, and in addition to the temperature gradient were combined for air and oxygen as an oxidizing agent and the results can be seen in Fig. 5. ER was ranged from 0.1 to 1.0 and temperature from 430 °C to 1000 °C. Equivalence ratio is proposed by [58,59] as follows:

$$ER = \frac{Air/Fuel\ Mass}{StoichiometricAir/Fuel\ Mass} \tag{17}$$

The air–fuel ratio is the ratio between the amount of air needed to complete combustion and the amount of fuel available. In this study, for a temperature of 700 °C, the air–fuel ratio ranged from 0.1 to 1.0, more air being allowed in the system to verify the influence of this parameter in syngas composition. The results of varying air–fuel ratios can be seen in Fig. 5 , which shows that the maximum value of CO_2 when air is the oxidizer is obtained when ER equals 1.

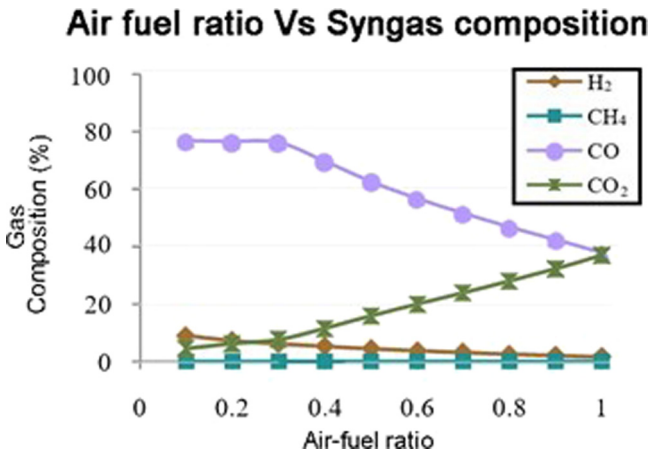

Fig. 5. Effect of air–fuel ratio (gasifier temperature: 700 °C).

From Fig. 5, it is observable that syngas quality is strongly affected by the air–fuel ratio, therefore influencing ER. For the range of studied values, when the air–fuel ratio increases from 0.3 to 1.0, CO_2 concentration increases by 30%, in contrast to CO, which drops by 35%. The concentration of H_2 decreased (from 10% to 2%), and CH_4 remained unchanged. Low air–fuel ratios tend to compromise the results, as incomplete gasification may occur, while on the other hand, high values for this parameter may promote the excessive formation of combustion products, such as CO_2 and H_2O, at the expense of fuel gases like H_2 and CO [22,23,28]. The results herein achieved are in accordance to these findings, as shown by the following trends: when air–fuel ratio increased, CO_2 yield rose, while CO and H_2 decreased, due to the oxidation reactions favored.

4.3. Temperature effect

Temperature is one of the chief operating variables for gasification, due to the endothermic nature of the main gasification reactions. The final gas composition reflects the result of complex and competing reactions, as for instance Boudouard reaction, water-gas and water-gas shift reactions, which are promoted by higher temperatures, according to Le Chatelier's principle. Fig. 6 shows the effect of temperature variation for an air–fuel ratio of 0.2.

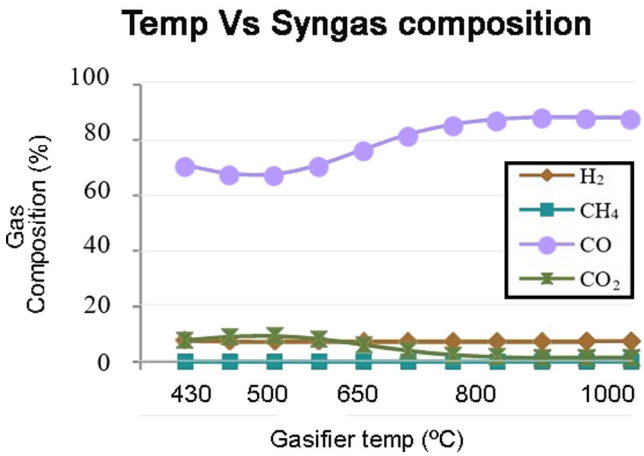

Fig. 6. Effect of gasifier temperature (air–fuel ratio: 0.2).

For the gasifier temperature ranging from 500 °C to 850 °C, the CO concentration increases by about 15% in the gasifier while the CO_2 is reduced by 15%, the H_2 concentration is the same for air and air/oxygen as the oxidants, but the amount of H_2 in the synthesis gas is greater when using air as the oxidant. This can be explained because more oxygen consumes H_2 and converts it to CO according to the water-gas shift and methanation reactions. It was also found that the concentrations of CH_4 have remained constant. Other authors report a similar trend for CO_2 content, explaining that it was consumed by the Boudouard and tar reforming reactions [22,23,28]. In addition, at higher temperatures, the exothermic water gas shift reaction promotes the formation of H_2O and CO, lowering the yield of CO_2.

5. Conclusion

With the present work, a kinetic model (phenomenological model more robust than a chemical equilibrium model) was developed for gasification to process different types of solid waste. This was done to promote the transformation of residues in a combined energy generation cycle, as a strategy to reassess waste, keeping its added value for a much longer period (Closed Chain Life Cycle), instead of disposing it in landfills, as recurring end-of-life scenario. This work contributes to the search for sustainable alternatives, actions that have been gaining notoriety and are increasingly recommended by government and administrative bodies, as they promote the efficient use of resources. In this way, waste is no longer considered 'garbage', becoming a raw material for other processes and being reintegrated into a clean energy production chain. This promotes the "closing the loop" approach, as preconized by circular economy principles.

The proposed mathematical model allowed a detailed analysis, considering the partial derivatives as a function of space and time of the modeled system, using applications with CFD tools. A fixed bed gasifier was simulated using EMSO software for solid waste gasification, a dedicated subroutine involving solid phases being implemented, to enhance feedstock flexibility for a wider range of materials. This work is an initial step in syngas production and recovery chain. As an impact of this work, we highlight the construction and contribution of knowledge to this framework, which proved to be very useful, as circular strategies for sustainable development.

The model presented results compatible with the experimental data in the literature and could also simulate other compositions of MSW and biomass. However, one of the main limitations found in the simulation is the sensitivity, which requires a precise adjustment of the diffusion and heat exchange parameters. A fundamental aspect to consider was the fact that pyrolysis reactions are fundamental for a good prediction of the composition profiles of the generated gases, since they characterize the fraction of components in which the biomass decomposes thermally. Therefore, a good adjustment of the kinetic parameters for the pyrolysis reactions was essential for a good correlation with the experimental data. Another limitation was the approach of the process by a one-dimensional model, as it greatly restricted the representation of multiple injections of lateral airflow along the gasifier. Using the

model, the impact of parameters such as air–fuel ratio, gasifier temperature and moisture content can be estimated over the entire operation. Other studies are being carried out to model the performance of gasification and optimize its operating conditions, using different raw materials such as agricultural and forestry residues. The presented results are preliminary and are still under analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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