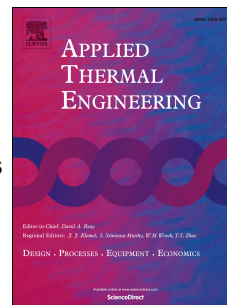


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Numerical and Experimental Analysis of Municipal Solid Wastes Gasification**Process**

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Abstract

As the quantity of municipal solid waste (MSW) increases with economic growth, problems arise in regard to sustainable management solutions. Thermal treatment presents a valid option for reducing the amounts of post-recycling waste to be landfilled. Incineration technology, besides reducing the total volume of waste and making use of the chemical energy in MSW for power generation, has negative environmental impact from high emission of pollutants. Recent policy to tackle climate change and resources conservation stimulated the development of renewable energy and landfill diversion technology, thereby giving gasification technology development renewed importance. In this work a two-dimensional CFD model for MSW gasification was developed and an Eulerian-Eulerian approach was used to describe the transport of mass, momentum and energy for the solid and gas phases. This model is validated using experimental data from the literature. The numerical results obtained are in good agreement with the reported experimental results.

Keywords: Gasification, municipal solid wastes, CFD, Eulerian-Eulerian approach

1. Introduction

The amounts of municipal solid waste (MSW) produced increase with economic growth in both industrialised and developed countries, raising the issue of sustainable management solutions [1].

MSW management activities contribute to the generation of greenhouse gas and consequently to the climate change problem. Landfill waste decomposition contributes greatly to the formation of these gases [2-5]. Another environmental problem associated with MSW management systems is the potential generation of dioxins and furans associated to complete combustion of wastes [2].

Thermal treatments are a valid option for reducing the amounts of post-recycling waste to be landfilled, which is considered to be one of the most sanitary disposal methods [3].

It should be noted that biogas production is not an alternative to thermal treatments like incineration or gasification because biogas is produced from the organic fraction of MSW and thermal treatment is applied to the non-organic, non-recyclable fraction [4].

In theory, gasification is a more suitable technology even where the market for thermal product is difficult, however the constraint with gasification of MSW is the technology which is not yet proven at commercial scale. [4]

Raw MSW contains a large amount of non-combustible material, and therefore requires pre-processing before sending it to a gasifier. The pre-processing must be able to meet the requirements of the gasifier and be flexible enough to handle MSW variability. This flexibility must be in terms of the type of material handled and its frequency of delivery. The pre-processing area is assumed to be similar to a Refuse Derived Fuel (RDF)

facility. Some recyclables and non-combustibles are removed from the MSW to make a higher heating value product that is sized appropriately for gasification [5]. Therefore, incineration continues to be the most common method of thermal treatment for waste-to-energy facilities. However, with the enhancement of environmental restrictions and the development of gasification technology, gasification presents an increasingly efficient and viable alternative to incineration. Gasification is a waste-to-energy conversion scheme that offers a most attractive solution to both waste disposal and energy problems. However, gasification still has some economic and technical challenges, concerning the nature of the solid waste residues and its heterogeneity [4-6]. The greatest strength of gasification is the environmental performance, since emission tests indicate that gasification meets the existing limits and it can also have an important role in the reduction of landfill disposal [3].

Incineration reduces the initial volume of the waste by as much as 85% and offers solutions for problems such as waste odour and leachate. The incineration process creates a large amount of solid residues which are divided into bottom ash and fly ash. Bottom ash represents 85–90% of the total ash produced and is collected at the base of the combustion chamber. This type of ash consists primarily of coarse non-combustible material, unburned organic matter and grate siftings [7]. These are disposed of in sanitary landfills. Fly ash are finely divided particles of ash which are normally entrained in the combustion gases. Fly ash is recovered from the gas stream by a combination of precipitators and cyclones. Incineration technology was developed to reduce the total volume of waste and make use of the chemical energy of MSW for energy generation. However, the incineration process also creates high emissions of pollutant species such as NO_x, SO_x, HCl, as well as harmful organic compounds and

heavy metals. Another problem with MSW incineration is corrosion of the incineration system by alkali metals in solid residues and fly ash [8].

Recent policies to tackle climate change and resource conservation such as the Kyoto Protocol, the deliberations at Copenhagen in 2009 and the Landfill Directive of the European Union have stimulated the development of renewable energy and landfill diversion technology, thereby giving the development gasification technology renewed importance [9].

Gasification is a thermochemical process that involves the oxidation of matter using a fraction of oxidizing agent in low quantities, inferior to the stoichiometric need. Gasification is considered an efficient and environmentally friendly way of extracting energy from different sources of organic materials [10]. Various studies [4-5, 11-13] pointed out that gasification is an emerging but promising technology, especially when compared with commercially-available technologies, such as direct combustion. For instance, Murphy and McKeogh [4], Jones et al. [5] and Lymberopoulos [11], suggested that gasification has better performance, e.g. higher electrical and overall efficiency, lower emissions and lower investment costs than direct combustion. Boustouler and Reynolds [12] corroborates with Lymberopoulos [11] in this regard but also claimed that reduced slagging problems is another advantage of gasification. Roos [13] discussed in more details environmental benefits of biomass gasification, including (i) reduced carbon emissions as a result of improvement in energy efficiency and char addition to soils, (ii) reduced use of fertilizers and runoff of nutrients from soils amended with char-containing ash, and (iii) reduced NO_x emissions due to better control of the combustion process.

The environmental performance is one of the greatest strengths of gasification technology, which is often considered a comprehensive response to the increasingly restrictive regulations applied around the world [4,9]. Independently-verified emissions tests indicate that gasification is able to meet existing emissions limits and can have a great effect on the reduction of landfill disposal option. Economic aspects are probably the crucial factor for a relevant market penetration, since gasification-based plants tends to have ranges of operating and capital costs about 10% higher than those of conventional combustion-based plants [9]. This is mainly a consequence of the ash melting system and the added complexity of the technology.

The technical challenges to overcome for a wider market penetration of commercial advanced gasification technologies can be investigated with the development of numerical simulation methods validated with experimental results of MSW gasification.

Gasification involves a set of fairly complex phenomena such as heat and mass transfer, fluid dynamics, and different chemical reactions. Numerous approaches to modelling gasification in CFD [14-19] and non-CFD [20-24] have been made. Currently there are three numerical techniques used for the studying gasification in fluidized beds in literature and these are Eulerian- Lagrangian with single particle or a particle parcel and a group of particles, Eulerian-Eulerian Two Fluid Model and Discrete Element Method within Eulerian-Lagrangian concept [14]. Literature concerning the numerical modelling of fluidized bed gasifier could be divided into three parts based on the geometric regions of fluidized bed furnace. It is dense bed, splash zone and freeboard/riser of fluidized bed units. Regarding dense bed most of studies are done with Eulerian- Eulerian Two Fluid Model approach [19]. Most of the literature in fluidized bed gasification is overlooking three-dimensional behaviours [14].

Cornejo and Farías [15] developed three-dimensional numerical model that describes the process of coal gasification in fluidized-bed reactors using an Eulerian-Eulerian approach. The main contribution of this work was implementing some sub-models within the FLUENT code in order to handle reactive fluidized-beds in complex geometries.

Xie et al [16] developed a three-dimensional numerical model to simulate forestry residues gasification in a fluidized bed reactor using an Eulerian–Lagrangian approach. The model predicts product gas composition and carbon conversion efficiency in good agreement with experimental data.

Baliban et al. [17] proposed an approach for modeling of a biomass gasifier which is validated for lignocellulosic type of biomass with experimental data.

Onel et al. [18] presents a generic gasifier model towards the production of liquid fuels using municipal solid wastes. Using a nonlinear parameter estimation approach, the unknown gasification parameters are obtained to match the experimental gasification results. The results suggest that a generic MSW gasifier mathematical model can be obtained in which the average error is 8.75%.

Silva et al. [19] developed a two-dimensional Fluent based model to simulate the gasification of agro-industrial residues. The numerical simulation results were compared and validated versus a set of runs using three kind of biomass residues that were gasified in a bubbling fluidized pilot scale unit. Their results are in good agreement with the experimental data obtained at three different operating conditions.

Thermodynamic equilibrium models are very useful tools to study the influence of most parameters for any biomass system because of their gasifier design independence. In

general, the thermodynamic equilibrium models consider two approaches both giving the same results: the stoichiometric approach, which requires a clearly defined reaction mechanism that incorporates all chemical reactions and species involved, and the non-stoichiometric approach which is based on the system minimization of the Gibbs free energy [20]. Several equilibrium models have been used to predict syngas composition from different biomass substrates [20-24].

The aim of this paper is to analyse MSW gasification using a numerical method. A two-dimensional mathematical model was developed using an Eulerian-Eulerian approach to model the MSW gasification in a fluidized-bed reactor within Fluent [25]. The model takes detailed chemistry into account as homogeneous reactions for the gaseous phase and heterogeneous reactions to the solid phase, and also the modelling of heat and mass transfer and momentum. Pyrolysis is included considering a model with generation of secondary tar. The choice of a fluidized bed reactor is due to the fact that is widely used in industry for converting coal and there is a good understanding of pyrolysis and gasification in this kind of reactor. Fluidized beds are also capable of being scaled up to medium and large scale, overcoming limitations found in smaller scale, fixed-bed designs [26]. In order to validate the numerical results obtained in this work we refer to an experimental study on MSW gasification and melting technology conducted by Xiao et al. [27].

2. Materials and Methods

2.1 Description of Portuguese waste management

The Portuguese MSW management system involves collection, storage, treatment and disposal as shown in the Fig. 1.

There are two possible routes for wastes collection - the selected and unselected wastes collection. The selected collection includes ecopoints and door-to-door collection with ecocentres and biodegradable municipal waste collection. Ecopoints are devoted to separate collection based on the use of different containers for glass, paper/cardboard, and plastic/metal, placed together at ecopoints preferably located on public thoroughfares and strategic points. Ecocentres are sorting centres, where the selected wastes from the ecopoints are delivered for recovery. In addition to the materials referred to above as part of mechanical recycling, there are other specific fluxes of wastes (used oils, batteries, electrical and electronic wastes, construction and demolition residues, end-of-life vehicles and used cooking oil).

The unselected collection is devoted to the collection of raw MSW. Raw MSW contains a large amount of non-combustible material, and therefore requires pre-processing before sending it to a gasifier. This pre-processing is made in the so-called mechanical and biologic treatment (MBT) station, where the biodegradable waste and the recyclable wastes are separated reducing the amount of waste to landfill.

They must be able to meet the requirements of the gasifier and be flexible enough to handle MSW variability. This flexibility must be in terms of the type of material handled and its frequency of delivery.

This pre-processing area is assumed to be similar to a Refuse Derived Fuel (RDF) facility. Some recyclables and non-combustibles are removed from the MSW to make a higher heating value product.

Transfer stations provide the facilities required for unselected wastes when landfills or the mechanical biological treatment (MBT) station are far away. Therefore, unselected

collection can be understood as the sum of landfill wastes with energetic and organic refuse.

MBT plants are designed to process mixed household wastes as well as commercial and industrial wastes. The MBT tolerates recycling paper, metal, plastic and glass. It can produce RDF or stabilize the biodegradable materials by composting or anaerobic digestion.

Biodegradable wastes can be converted into compost, carbon dioxide and water under an aerobic process. Composting is the common process for organic recovery of the wastes into soil conditioner. The remaining non-biodegradable wastes are recycled to recover materials for new products [28].

The RDF can be further used as alternative fuel in cement kilns or incinerated to produce energy. The ash formed during incineration contains mostly inorganic constituents of the wastes and is often landfilled [28].

Wastes from unselected collection as well as waste coming from MBT, incineration plants, composting and recycling refuse are disposed of in landfills. Landfilling is the last treatment to be adopted because it causes severe environmental impact from greenhouse gases released into the atmosphere and also from leachate percolating into ground water. To help minimize the environmental impact, the biogas generated by anaerobic reactions can be used as fuel to produce heat and power [29].

2.2 Standard Municipal solid waste characterization

MSW increases significantly in industrialized and developing countries, raising questions about sustainable municipal solid waste management. This results from the

collection of waste in large urban areas, and comprises materials such as household waste, plastic, paper, glass, metals, and garden waste [30]. The composition of municipal solid waste depends on both the season and geographic location. The heterogeneous nature of the wastes affects the physical properties in terms of size, elemental composition, moisture content, heating value, ash content, volatile content and other contaminants. Therefore, the wastes are pre-treated accordingly to the Portuguese management system described previously.

Lipor is the entity responsible for the management, treatment and recovery of MSW in the Oporto metropolitan area. This includes eight municipalities in the Oporto metropolitan area and a production of about 500,000 tons/year of MSW by 984,047 inhabitants [31]. During the year 2012 Lipor carried out two sampling campaigns in the winter and in the summer. A criteria analysis of the waste collected was held, and the physical characterization by categories is shown in Table 1.

As an outcome of the pre-treatment defined previously results a RDF which contains cellulosic materials and plastics due to putrefied wastes, paper, wood wastes, and plastic residues. The remaining MSW components follow another route for valorization or elimination. It has been shown that the plastic residues are mainly composed of polyethylene, polystyrene, and poly-vinyl chloride [32] and the cellulosic materials are composed of cellulose, hemicelluloses, and lignin [17].

Given that the ultimate analyses of the Lipor does not distinguish the cellulosic materials, it was postulated that their composition was similar to the one found in [18], where the cellulosic material comprises cellulose, hemicellulose and lignin. Regarding the plastics group, Lipor report shows the relative quantities of each monomer in the

MSW. Therefore, it was possible to take into account different monomers for the plastics group as shown in Table 2.

To enable the use of Fluent code to perform the numerical simulations a global chemical formula of the MSW is necessary. This calculation was performed based on the chemical characterization of waste shown in Table 2. The fractions of carbon (C), hydrogen (H) and oxygen (O) are found by ultimate analysis of the mixture. The total carbon was the sum of the carbon in all the hydrocarbons. The same procedure is made for the calculation of the total hydrogen and total oxygen. This calculation is performed by dividing the values found in the ultimate analysis of each chemical element by the value of the reference element carbon (C).

3. Mathematical Model

The purpose of this section is to develop a modelling approach able to predict the final composition of the syngas resulting from gasification using numerical simulation. The improved state-of-the art CFD models enable the design and optimization of the gasification processes [33]. The numerical simulation was performed using the CFD solver Fluent based on finite volume method. The gasification was modeled using Fluent data base for a two-dimensional model and multi-phase (gas and solid) model. The solid phase was treated as an Eulerian granular model while the gas phase is considered as continua. The main interaction between the phases is also modeled, heat exchange by convection, mass (the heterogeneous chemical reactions), and momentum (the drag in gas and solid phase). In the next section the governing equations will be described.

3.1 Energy Conservation

The energy conservation equation for both phases (gas and solid) is as follows [34]:

$$\frac{\partial(\alpha_q \rho_q h_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \bar{u}_q h_q) = -\alpha_q \frac{\partial(\rho_q)}{\partial t} + \bar{\tau}_q : \nabla(\bar{u}_q) - \nabla \cdot \bar{q}_q + S_q + \sum_{p=1}^n (\bar{Q}_{pq} + \dot{m}_{pq} h_{pq} - \dot{m}_{pq} h_{pq}) \quad (1)$$

Where \bar{Q}_{pq} is the heat transfer intensity between fluid phase p^{th} and solid phase q^{th} , h_q the specific enthalpy of phase q^{th} , \bar{q}_q the heat flux, S_q is a source term due to chemical reactions and h_{pq} the enthalpy of the interface.

Equation (2) [35] describes the rate of energy transfer as a function of the temperature difference between the phases; where the heat transfer coefficient between the phases

$$Q_{pq} = h_{pq}(T_p - T_q) \quad (2)$$

p^{th} and q^{th} is given by h_{pq} .

The heat transfer coefficient is associated to the Nusselt number of solid phase q^{th} , and k_p is the thermal conductivity for phase p^{th} [33]:

$$h_{pq} = \frac{6k_p \alpha_q \alpha_p Nu_q}{d_p^2} \quad (3)$$

Nusselt number is correlated by [35]:

$$Nu_q = (7 - 10\alpha_g + 5\alpha_g^2)(1 + 0.7 Re_s^{0.2} Pr_g^{0.33}) + (1.33 - 2.4\alpha_g + 1.2\alpha_g^2) Re_s^{0.7} Pr_g^{0.33} \quad (4)$$

where Re_s is the Reynolds number based on the diameter of the solid phase and the relative velocity, Pr_g is the Prandtl number of the gas phase.

3.2 Momentum Model

The gas and solid phase momentum equations are as follow: Equation (5) refers to solid phase momentum equation, t_s are the particle phase stress tensor and P_s is the particle phase pressure due to particle collisions. The equation (6) represents the gas phase momentum equation, where β is the gas-solid interphase drag coefficient, τ_g the gas phase stress tensor and U_s the mean velocity of solid [34].

$$\frac{\partial}{\partial t}(\alpha_s \rho_s v_s) + \nabla \cdot (\alpha_s \rho_s v_s v_s) = -\alpha_s \nabla p_s + \alpha \rho_s g + \beta(v_g - v_s) + \nabla \cdot \alpha_s \tau_s + S_{sg} U_s \quad (5)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g v_g) + \nabla \cdot (\alpha_g \rho_g v_g v_g) = -\alpha_g \nabla p_g + \alpha \rho_g g + \beta(v_g - v_s) + \nabla \cdot \alpha_g \tau_g + S_{gs} U_s \quad (6)$$

3.3 Mass Balance Model

The biomass feed changes from solid phase into gas phase by reacting with oxygen, steam and carbon dioxide. The continuity equations for solid and gas phases are given by the equations (7) and (8), respectively [34].

$$\frac{\partial}{\partial t}(\alpha_s \rho_s) + \nabla \cdot (\alpha_s \rho_s v_s) = S_{sg} \quad (7)$$

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g v_g) = S_{gs} \quad (8)$$

where v is the instantaneous velocity of gas/solid phase, ρ the density and α the volume fraction, the subscripts s denotes the solid phase and subscripts g the gas phase. The mass source term due to heterogeneous reaction, S is expressed by the following equation:

$$S_{sg} = -S_{gs} = M_c \sum \gamma_c R_c \quad (9)$$

In which R_c is the reaction rate, γ_c the stoichiometric coefficient and M_c the molecular weight. The solid phase density was assumed to be constant. The gas phase density was calculated on the basis of ideal gas equation:

$$\frac{1}{\rho_g} = \frac{RT}{p} \sum_{i=1}^n \frac{Y_i}{M_i} \quad (10)$$

Where R is the universal gas constant, T the temperature of the gas mixture, p the gas pressure, Y_i the mass fraction and M_i the molecular weight of each the species.

3.4 Turbulence Model

A Fluent standard k- ϵ model was chosen for the turbulence model, as this is the most appropriate model when turbulence transfer between phases plays an important role in gasification in fluidized beds. k is the turbulence kinetic energy and ϵ is the dissipation rate. They are determined by the next transport equations [36]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \right] + G_k + G_b - \rho \epsilon - Y_M + S_k \quad (11)$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_j}(\rho \epsilon u_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} \rho \frac{\epsilon^2}{k} + S_\epsilon \quad (12)$$

From Eq. (11) G_k is the generation of turbulence kinetic energy due to the mean velocity gradients, G_b the generation of turbulence kinetic energy due to buoyancy, and Y_M the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate. In the Eq. (12) $G_k = 1.0$ and $G_\epsilon = 1.3$ are the turbulent Prandtl numbers for k and ϵ , respectively, S_k and S_ϵ are user-defined source terms. $C_{1\epsilon} = 1.44$, $C_{2\epsilon} = 1.92$, and $C_{3\epsilon} = 0$ are constants suggested by Launder and Spalding [35].

3.5 Granular Eulerian Model

Granular Eulerian model is described by the following conservation equation for the granular temperature [37]:

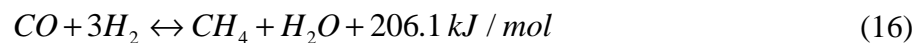
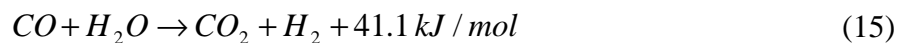
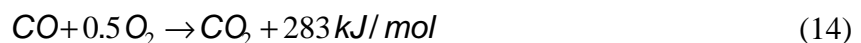
$$\frac{3}{2} \left[\left(\frac{\partial(\rho_s \alpha_s \Theta_s)}{\partial t} + \nabla \cdot (\rho_s \alpha_s \vec{v}_s \Theta_s) \right) \right] = (-P_s \bar{I} + \bar{\tau}_s) : \nabla(\vec{v}_s) + \nabla \cdot (k_{\Theta a} \nabla(\Theta_s)) - \gamma_{\Theta a} + \phi_{Is} \quad (13)$$

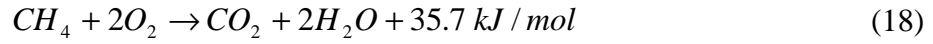
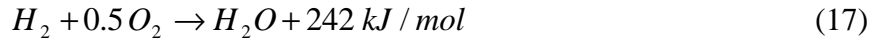
This equation is obtained from the kinetic theory of gases. The term $(-P_s \bar{I} + \bar{\tau}_s) : \nabla(\vec{v}_s)$ describes the generation of energy by the solid stress tensor, ϕ_{Is} is the energy exchange between the fluid phase and the solid phase, $\gamma_{\Theta a}$ the collisional dissipation of energy and $k_{\Theta a} \nabla(\Theta_s)$ the diffusion energy ($k_{\Theta a}$ is the diffusion coefficient).

The stress in the granular solid phase is achieved by relating the random particle motion and the thermal motion of molecules within a gas accounting for the inelasticity of solid particles. In a gas the intensity of velocity fluctuation determines the stresses, viscosity and pressure of granular phase.

3.6 Chemical Reactions Model

The chemical reaction rate coefficients are based on the Arrhenius law. Actually, they are empirical and determined by fitting the experimental data. During the devolatilization and cracking water shift reaction will occur, the gas species react with the supplied oxidizer and among them. The most common homogenous gas-phase reactions are [38]:





The Arrhenius rates for each one of these reactions can be expressed as follows, respectively [39, 40]:

$$r_{CO_Combustion} = 1.0 \times 10^{15} \exp\left(\frac{-16000}{T}\right) C_{CO} C_{O_2}^{0.5} \quad (19)$$

$$r_{H_2Combustion} = 5.159 \times 10^{15} \exp\left(\frac{-3430}{T}\right) T^{-1.5} C_{O_2} C_{H_2}^{1.5} \quad (20)$$

$$r_{CH_4Combustion} = 3.552 \times 10^{14} \exp\left(\frac{-15700}{T}\right) T^{-1} C_{O_2} C_{CH_4} \quad (21)$$

$$r_{water_gas_shift} = 2780 \exp\left(\frac{-1510}{T}\right) \left[C_{CO} C_{H_2O} - \frac{C_{CO_2} C_{H_2}}{0.0265 \exp\left(\frac{3968}{T}\right)} \right] \quad (22)$$

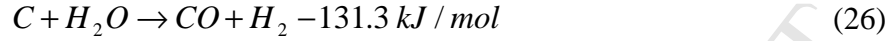
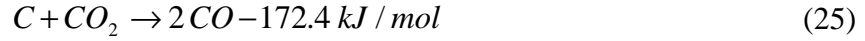
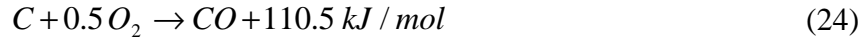
The Eddy dissipation reaction rate can be expressed using the following equation [25]:

$$r_{Eddy-dissipation} = \alpha_{i,r} M_{w,i} A \rho \frac{\varepsilon}{k} \min\left(\min_R \left(\frac{Y_R}{\alpha_{R,r} M_{w,R}} \right), B \frac{\sum_p y_p}{\sum_i \alpha_{i,R} M_{w,i}} \right) \quad (23)$$

The minimum value of these two contributions can be defined as the net reaction rate.

The heterogeneous reactions of char (the solid devolatilization residue) with the species O_2 and H_2O are very complex processes. They demand a mass diffusion balance of the oxidizing species at the surface of the biomass particle with the surface reactions of those species with the char. The composition and the temperature of the gases, as well as the temperature, size and porosity of the particle are important to determining the overall rate of the char.

The most used overall simplified heterogeneous reactions are [38]:



The heterogeneous reactions are influenced by many factors, namely, reactant diffusion, breaking up of char, interaction of reactions and turbulence flow. In order to include both diffusion and kinetic effects the Kinetic/Diffusion Surface Reaction Model [41] was applied. This model weights the effect of the Arrhenius rate and the diffusion rate of the oxidant at the surface particle. The diffusion rate coefficient can be defined as [25]:

$$D_0 = C_1 \frac{[(T_p + T_\infty) \div 2]^{0.75}}{d_p} \quad (27)$$

The Arrhenius rate can be defined as follows:

$$r_{Arrehnus} = A e^{-\left(\frac{E}{RT_p}\right)} \quad (28)$$

The final reaction rate weights both contributions and is defined as follows [25]:

$$\frac{d_{m_p}}{d_t} = -A_p \frac{\rho R T_\infty Z_{ox}}{M_{w,ox}} \frac{D_0 r_{Arrehnus}}{D_0 + r_{Arrehnus}} \quad (29)$$

This model was included in the CFD framework by using the User Defined Function tool.

3.6.1. Pyrolysis

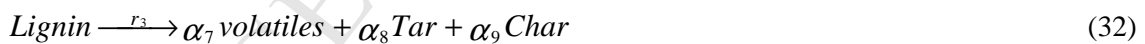
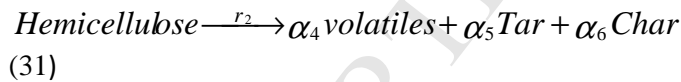
Both homogeneous and heterogeneous reactions are preceded from pyrolysis reactions. Modeling pyrolysis is crucial for MSW gasification purposes.

MSW is thermal decomposed into volatiles, char and tar. There are several approaches to describe this phenomenon and 3 main approaches are usually followed: a single step pyrolysis model, competing parallel pyrolysis and a pyrolysis model with generation of secondary tar.

In this model we adopt a pyrolysis model with generation of secondary tar. The MSW is mainly composed by cellulosic and plastic components, where the cellulosic material can be divided in cellulose, hemicellulose and lignin [17, 18] and the plastics are mainly comprised by polyethylene, polystyrene, and polypropylene, among others.

To distinguish the several components that comprise the MSW, the pyrolysis reactions of cellulosic and plastic groups are considered individually and following an Arrhenius kinetic expression.

The primary pyrolysis equations can be defined as follows:



The kinetics for the cellulosic material can be given as follows:

$$r_i = \frac{d a_i}{dt} = A_i \exp\left(\frac{-E_i}{T_s}\right) (1 - a_i)^n \quad (34)$$

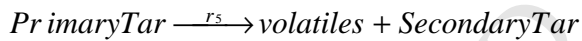
Where i stands for cellulose, hemicellulose and lignin (r_{1-3}), A_i is the pre-exponential factor, E_i is the activation energy and n is the order reaction. The values for each one of these parameters can be found in [42]. Average values were considered.

Regarding the kinetic reactions for plastics, data was obtained from [43] by using the following reactions:

$$r_4 = \left[\sum_{i=1}^n A_i \exp\left(\frac{-E_i}{RT}\right) \right] \rho_v \quad (35)$$

Where A_i , E_i and ρ_v are the pre-exponential factor, the activation energy and the volatiles density, respectively, and can be found in [43]. i stands for each one of the plastics that comprise the analyzed MSW along this paper.

In this model, it is considered a secondary pyrolysis where is generated volatiles and secondary tar, as follows:



Because, this secondary pyrolysis is also very difficult to treat, a simplified global reaction is used [44]:

$$r_5 = 9.55 \times 10^4 \exp\left(\frac{-1.12 \times 10^4}{T_g}\right) \rho_{Tar1} \quad (36)$$

3.7 Numerical procedure

The simulations were performed in an up-flow atmospheric fluidized bed gasifier. This fluidized bed reactor is a tubular reactor of 0.5 m in diameter and 4.15 m of height, internally coated with ceramic refractory materials; MSW enters the reactor at the height of 0.5 m, from its base, and preheated air at 600 K enters the reactor coming from

the base through a set of diffusers, warranting a flow of about $70 \text{ m}^3/\text{h}$. The schematics of the fluidized reactor are depicted in Fig. 2 and the bed is made of 70 kg of dolomite.

The problem under consideration is solved by using a finite volume method based CFD solver FLUENT. The unstructured quadrilateral cells of non-uniform grid spacing are generated using GAMBIT. The grid is chosen to be sufficiently fine to capture the steep gradients in the vicinity of the cylinder. The second order upwind scheme is used to discretize the convective terms in the momentum and energy equations. The SIMPLE scheme is used for solving the pressure-velocity coupling. The system of algebraic equations is solved using the Gauss-Siedel point-by-point iterative method in conjunction with the algebraic multi-grid method solver. Relative convergence criterion for residuals of 10^{-8} was prescribed in this work.

4. Results and discussion

Despite having sparse data about municipal solid waste gasification in semi-industrial or industrial facilities, experimental data about MSW gasification in China was gathered from the literature [27]. Based on the characteristics of MSW from China, raw materials were prepared according to the average proportion of organic components (dry basis) for gasification, as displayed in Table 3.

In order to perform simulations with the Xiao MSW composition [27] using Fluent code, a global chemical formula is needed. Using the same procedure that was used and described for Lipor MSW and assuming that kitchen garbage, wood and yard waste, paper and textile, are assumed to be cellulosic materials, and the plastics materials with the same relative composition of the Lipor MSW, the global chemical formula is obtained.

4.1 Model validation

In order to validate the mathematical model proposed previously, numerical simulations were carried out using the Xiao MSW. The results obtained numerically were compared with the experimental results of Xiao et al. [27]. The results of run 1 are shown in Fig. 3 for the gasification conditions defined in Table 4. Relative errors between numerical and experimental results are depicted in Table 5. The relative error is computed as follows:

$$\text{Relative error (\%)} = \frac{(\text{numerical value} - \text{experimental value})}{\text{experimental value}} \times 100\% \quad (37)$$

The model estimates reasonably all the species in a large spectrum of operating conditions. The largest errors are found for species at minor molar fractions. Despite these numerical results being within the range of values of the experimental results, there are still a few deviations which are justified by some simplifications performed, such as: i) The lack of data on the characteristics of waste has led to the use of constants of other biomasses which may differ from the actual one, ii) The kinetic constants were taken from the literature and can differ greatly from source to source.

4.2 Results of Lipor MSW gasification

After validating the numerical model, numerical simulations were carried out and the results obtained for syngas gasification of Lipor's MSW are shown in Fig. 4 for the gasification conditions defined in Table 6.

These results are within the range of literature results [45, 46].

Figure 5 shows the contours of the H₂, CH₄, CO₂, and CO mole fractions in the gas mixture.

The highest values for CO₂ are located at the syngas outlet, which is consistent with the results of Qingluan and Rodney [45] and Oevermann et al. [46]. CO shows the opposite trend.

For CH₄ its higher value is found immediately above the biomass inlet, where the reduction phase takes place and these gases are formed, which is consistent with the results of Qingluan and Rodney [45].

The values of N₂ are not shown because are closely constant throughout the gasifier due to the unreacted characteristics of this gas, besides its possible combination with oxygen at high temperatures. This behaviour is also consistent with the results of Qingluan and Rodney [45].

The MSW collected by Lipor is representative of a population of 984,047 inhabitants, for a total of 500,000 tonnes of urban solid waste per year. Based on the numerical results of the gasification, it is possible to compute the production of 7.8×10^8 m³ of syngas during a year based on 500,000 tons of MSW.

This is a very interesting factor for Lipor incineration of waste. Lipor consumes about 20,000 m³ of natural gas per year to spray the waste before entry into the combustion chamber. Therefore, it could be advantageous for Lipor to consider replacing this natural gas with syngas resulting from municipal solid waste gasification.

5. Conclusion

In this work, we have modelled gasification as an alternative incineration process for energy recovery from MSW. A two-dimensional mathematical model was developed using the fluent code. An Eulerian-Eulerian approach was used to describe the transport of mass, momentum and energy for the solid and gas phases. The model was tested using gasification experimental data from the literature. The model reproduces the key features of municipal solid waste gasification. The numerical results achieved show reasonable agreement with the experimental results, with some deviations. Numerical simulations were made for the study of gasification of municipal solid waste from the North of Portugal, carried out particularly by Lipor, the entity responsible for the MSW management system in the Porto metropolitan area. These results agree partially well with the experimental data. The very heterogeneous nature of the MSW and the consequent variance of the properties such as elemental composition, density, water content, and structure leads to uncertainties in the modelling of MSW gasification, and should be kept in mind when comparing the numerical results with the experimental results.

For Lipor it would be interesting to consider using a gasification unit instead of the incineration. The associated production of syngas was estimated to be around 7.8×10^8 m³/year. However, a study of economic viability must be carried out, as well as optimization of the gasification process where the numerical simulation can give a valuable assistance.

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Nomenclature

$C_{1\varepsilon}, C_{2\varepsilon}, C_{3\varepsilon}$ Constants

C_p Specific heat capacity

G_k Generation of turbulence kinetic energy due to the mean velocity gradients

G_b Generation of turbulence kinetic energy due to buoyancy

d Hydraulic Diameter

g gravity acceleration

h_{pq} Heat transfer coefficient between the fluid phase and the solid phase

k Thermal conductivity

M_c Molecular weight

$M_{w,i}$ Molecular weight of i component

Nu Nusselt Number

\dot{m}_{pq} mass flow between the fluid phase and the solid phase

P_s	is the particle phase pressure due to particle collisions
p	Gas pressure
\vec{q}_q	Heat flux
q^{th}	Specific enthalpy
Q_{pq}	Heat transfer intensity between phases
R	Universal gas constant
R_c	Reaction rate
S	Mass source term due to heterogeneous reactions
S_k	User-defined source terms
S_q	Source term due to chemical reactions
S_ϵ	User-defined source terms
T	Temperature
U	Mean velocity
v	Instantaneous velocity
Y	Mass Fraction
Y_M	Contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate

Other Symbols

α Volume fraction

β Gas-solid interphase drag coefficient

ρ Density

ϕ_{is} Energy exchange between the fluid phase and the solid phase.

k_{θ_a} Diffusion coefficient

$k_{\theta_a} \nabla(\theta_s)$ Diffusion energy

$(-p_s \bar{I} + \bar{\tau}_s) : \nabla(\vec{v}_s)$ Generation of energy by the solid stress tensor.

γ_{θ_a} Collisional dissipation of energy

τ Tensor stress

μ Viscosity

γ_c Stoichiometric coefficient

Subscripts

g gas phase

s solid phase

i component

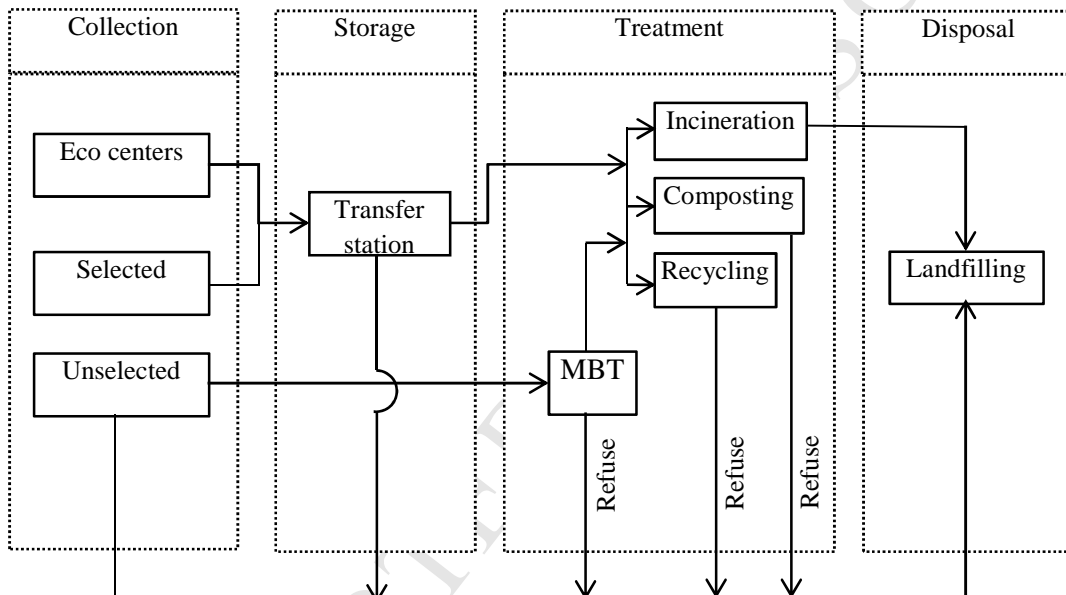


Figure 1- Schematic overview of the Portuguese waste management system [3].

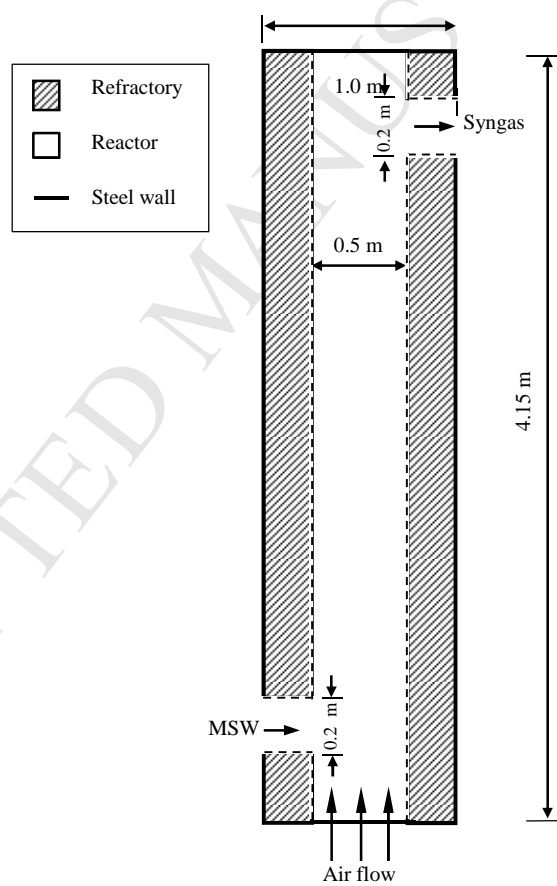


Figure 2 – Gasifier geometry

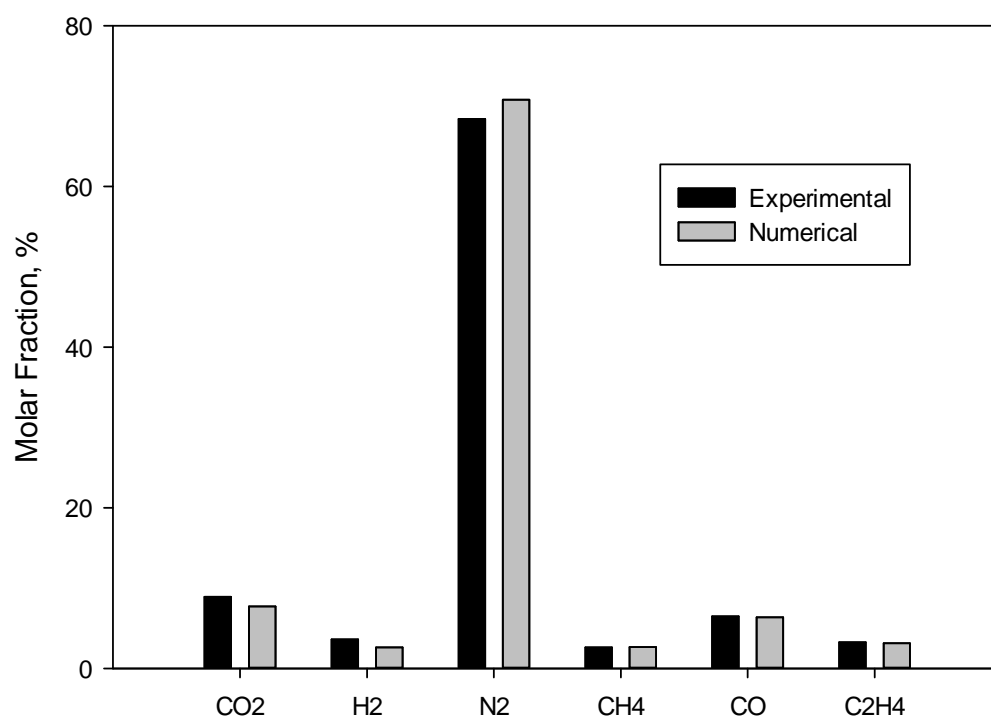


Figure 3 - Comparison of the CFD and experimental results for run 1 as defined in

Table 4.

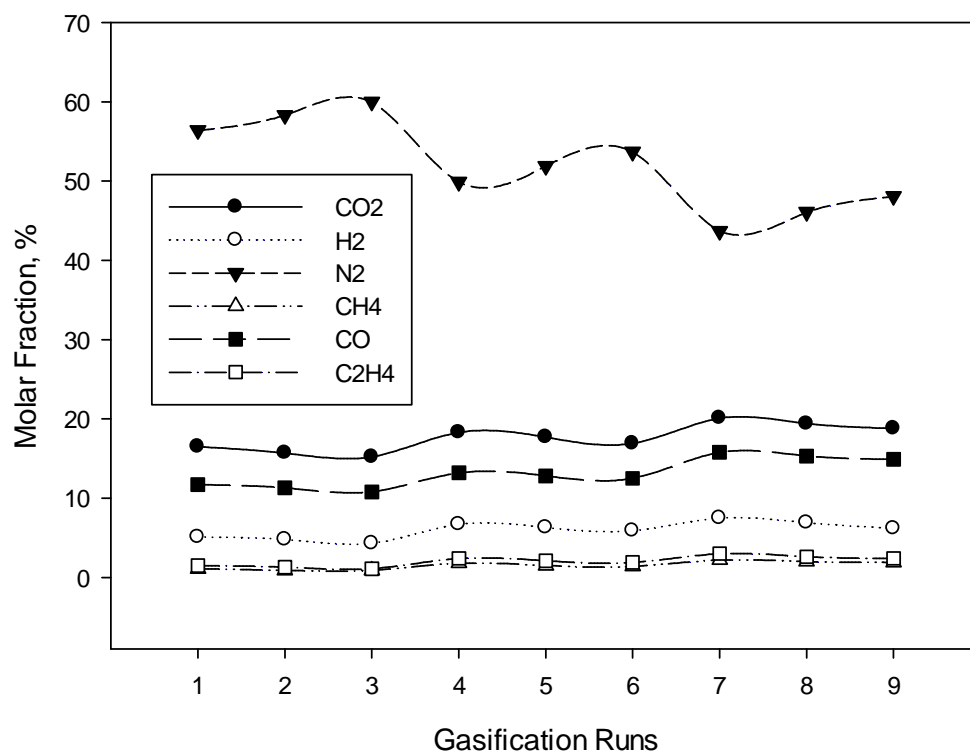


Figure 4 - CFD molar fractions of the Lipor MSW for 9 gasification conditions defined in Table 6.

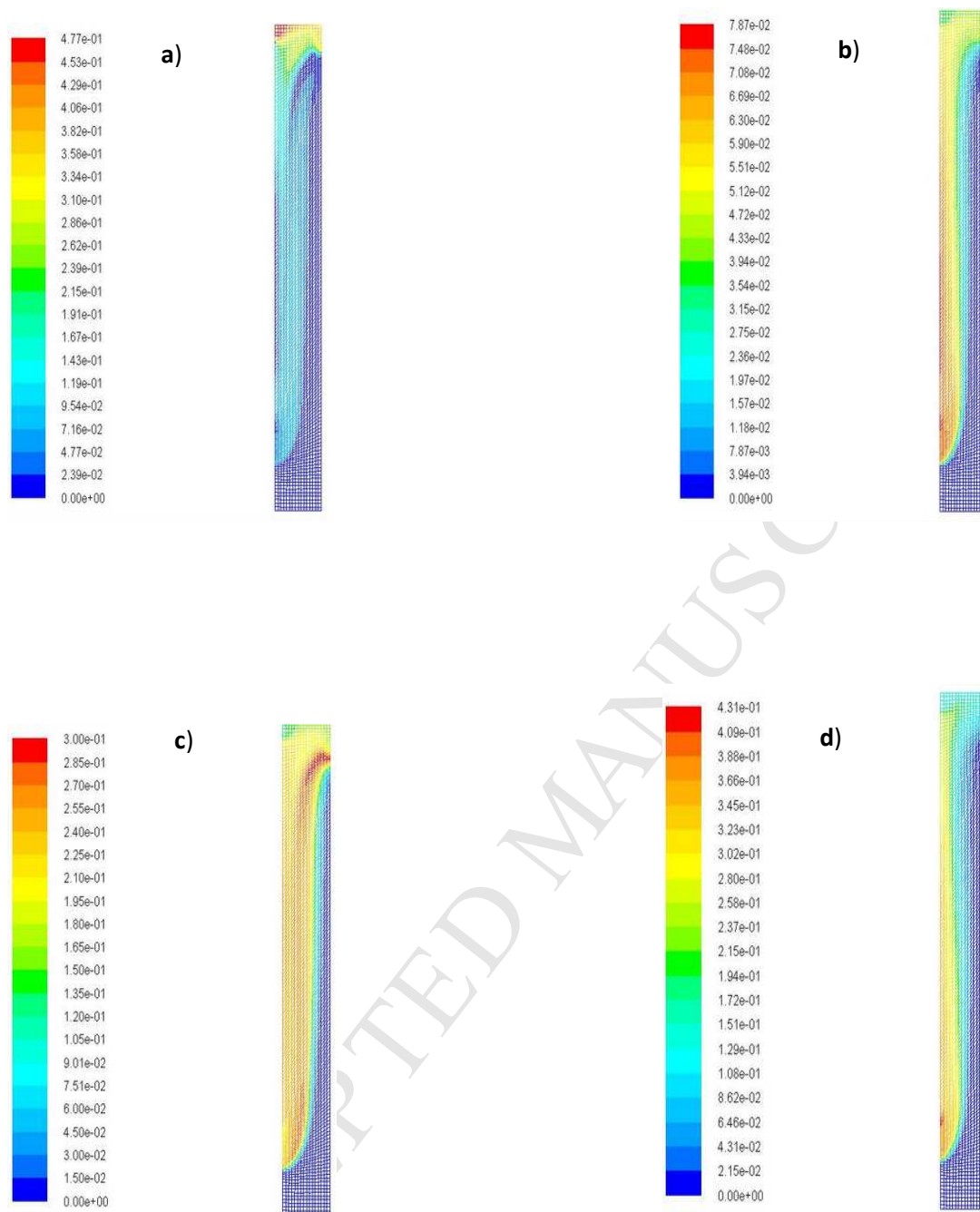


Figure 5 – Mole fraction contours for: (a) H₂, (b) CH₄, (c) CO₂, (d) CO.

Table1 – Physical characterization of the MSW [31].

Category	% weight
Putrefied residues	44.34%
Paper	4.74%
Cardboard	2.61%
Composites	4.68%
Textiles	5.73%
Sanitary textiles	1.20%
Plastics	10.98%
Combustive non specified	0.09%
Glass	4.29%
Metals	2.15%
Non-combustive non specified	0.41%
Hazardous residues	0.06%
Fine elements	8.72%

Table 2 - Chemical composition of the MSW.

Category	% weight	Chemical formula
Cellulosic material	85.22%	*
Polyethylene	11.14%	$(C_2H_4)_n$
Polyethylene terephthalate	2.05%	$(C_{10}H_8O)_n$
Polypropylene	0.82%	$(C_3H_6)_n$
Polystyrene	0.77%	$(C_8H_8)_n$

*It was considered the proportion of cellulose, hemicellulose and lignin found in [18].

Table 3 – Xiao et al. [27] MSW characteristics

Organic compounds (%)					
Kitchen garbage	Plastic	Wood and yard waste	Paper	Textile	Low heating value (kJ/kg)
61	20	10	8	1	17,960

Table 4- Experimental gasification conditions used for the model validation.

Gasification Run	Feeding rate of MSW (kg/h)	Flux of air (m ³ /h)	Temperature of gasification (°C)	Temperature of preheated air (°C)
1	2.3	6	720	352
2			620	283
3			493	290
4	3	6	705	352
5			602	296
6			507	281
7	4	6	687	352
8			593	307
9			516	282
10	6	6	691	352
11			593	308
12			507	279

Table 5- Relative error of the several syngas species along the 12 gasification runs.

Gasification Run	Relative error according to Equation (37) (%)					
	CO ₂	H ₂	N ₂	CH ₄	CO	C ₂ H ₄
1	-13.37	-27.50	3.54	1.92	-1.69	-3.70
2	1.88	-26.00	7.18	-27.14	-8.03	15.38
3	9.37	-8.57	3.32	-37.50	-6.04	10.81
4	3.95	7.86	6.88	11.84	3.60	9.25
5	4.14	-1.60	1.95	-14.44	-9.13	43.98
6	-6.08	8.00	1.62	-20.00	4.60	12.66
7	8.97	6.90	2.51	16.52	6.92	-8.12
8	4.04	9.63	2.07	-14.67	-5.33	0.92
9	3.62	27.27	2.54	-36.25	-3.40	43.56
10	4.17	-7.41	4.18	1.75	2.94	8.89
11	-1.29	-16.67	4.64	10.00	6.17	8.75
12	5.07	9.76	-3.41	13.89	6.42	29.63

Table 6- Gasification conditions for the Lipor MSW.

Gasification Run	Feeding rate of MSW (kg/h)	Flux of air (m ³ /h)
1	25	40
2		70
3		100
4	50	40
5		70
6		100
7	75	40
8		70
9		100

Highlights

- A multiphase 2-D model coupled with chemical reaction for MSW gasification.
- The numerical model is developed under the CFD Fluent framework.
- SYNGAS generation from biomass residues gasification is studied.
- Numerical and experimental (semi-industrial BFB gasifier) data are compared.

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