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Plasma gasification process using computational fluid dynamics modeling

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Abstract

The world has a waste problem. Landfills around the planet are reaching full capacity, so the recovery of energy from them would be a very useful green alternative and sustainable solution. A century-old technology is being revitalized to convert waste into energy through a process called plasma gasification. In this study, a proposed model of plasma gasification allows us the simulation of municipal solid waste (MSW) gasification and get the temperature field as well as the composition of the products (CO, CO₂, H₂, H₂O) inside the gasifier. It was found that the use of plasma greatly influence the quality of syngas. The temperature distribution showed that the updraft gasifier is actually operating at approximately 1000 K. It is well understood that increasing gasification temperature is beneficial since it enhances reaction rates, and influences the energy equilibrium of endothermic gasification. This emphasizes the importance of the current work because it depicts the various regions of the updraft reactor as well as the related gasification phases that occur in reality at different temperatures. Despite the good performance of the present model, it is necessary to develop it to improve the interaction of plasma flow with solid particles, liquids, or other gases.

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1. Introduction

The great challenge today is the depletion of natural reserves and the constantly rising prices caused by the world's high dependency on fossil fuels in the energy and transportation systems. This situation triggered considerable investigations on alternative energy sources to mitigate the world's high reliance on fossil fuels employing the waste-to-energy methodology. For these reasons, the demand for clean energy from renewable and sustainable energy have received much attention worldwide over the past decades. Since the early 90s, researchers

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Nomenclature

A_c	pre-exponential factor
CCE	carbon conversion efficiency
CFD	computational fluid dynamics
CGE	cold gasification efficiency
$c_{p\alpha}^0$	standard specific heat capacity
DC	direct current
d_p	particle diameter
$D_{t\alpha}$	thermal diffusion coefficient
$D_{m\alpha}$	mass diffusion coefficient
E_c	activation energy
ER	equivalence ratio
ε	dissipation rate of turbulent kinetic energy
g	gravitational force
G_k	generation of turbulent kinetic energy
HHV	higher heating value
h	specific enthalpy
IEA	renewable energy agency
k	turbulent kinetic energy
K_d	diffusion rate
k_{eff}	effective heat conductivity
LHV	lower heating value
MSW	municipal solid waste
μ	viscosity
p	static pressure
r	stress tensor
R_c	char consumption rate
Re	Reynolds number
ρ	density
Sc	Schmidt number
SBR	steam-to-biomass ratio
SIMPLE	semi-implicit method for pressure linked equations
T	temperature
UDF	user defined function
u_p	particle velocity
WtE	waste-to-energy
WtM	waste-to-material
ω	turbulent thermal conductivity
v	fluid velocity

have been embarking on research and development of thermochemical conversion processes that will play a critical role in alleviating the energy supply deficiency. The good news in these processes is that different material feedstocks (e.g. biomass, plastics, food waste, microalgae, and animal manure) can be used to yield high-end products or biofuels including hydrogen [1]. Producing clean hydrogen from renewable resources is nowadays considered as one of the most important green energy technologies, due to its high energy content and potential applications in power, chemical, and transportation sectors. Gasification is a proven technology to produce a satisfactory yield of hydrogen

[2]. On the other hand, plasma gasification has been regarded as a viable alternative for the treatment of highly toxic waste, such as the residue from MSW incineration (bottom ash + fly ash), radioactive, and medical wastes [3]. Various process parameters, such as reactor configuration, temperature, pressure, heating rate, retention time, reactive or inert environment, expulsion gas flow rate, use of catalyst, among others, can be employed to optimize the system and/or the quality of derived products [4–7]. Variable systems, type of plasma and design characteristics as well as limitations of the experimental conditions are the major causes concurring to a lack of consensus regarding this technique [5]. Experiments concerning both the optimization of operational conditions to predict syngas composition and quality, and the collection of experimental data to match the simulations are particularly important to adapt the developed models to the actual results and minimize the required resources. Due to the extensive range of investigations, mathematical and computational approaches have been applied to understand and predict the process behavior and to analyze effects of different variables on the process performance. Mathematical models have also the benefit of avoiding time-consuming and costly experimental procedures [8–11]. Different types of gasification mathematical models have been developed: thermodynamic equilibrium, kinetic, computational fluid dynamics (CFD), and artificial neural networks [12]. Although the modeling of plasma gasification is scarce in the literature, the most used types of mathematical models are the thermodynamic equilibrium and the CFD.

Mazzoni and Janajreh [13] conducted a thermochemical study of plasma co-gasification of MSW and plastic waste using Aspen Plus[®]. Their model validation study reveals that the developed model largely underestimates the methane molar fraction. Okati et al. [14] developed a thermodynamic equilibrium model in Aspen Plus[®] to perform a parametric study of the plasma gasification process of polychlorinated biphenyl wastes. Their results also indicate a high relative error in the prediction of the methane molar fraction. These are typical results of equilibrium models [12].

The CFD mathematical models are applied to plasma gasification for being more precise in their predictions [15]. Zhang et al. [16] developed an Euler–Euler model to simulate the plasma gasification of MSW using Ansys Fluent. The model considers the main chemical and physical processes and the melting of the inorganic components of MSW. The results indicate an optimal equivalence ratio (ER) of 0.6 for air gasification and for steam gasification a steam-to-waste ratio lower than 0.28. Ibrahimoglu et al. [17] modeled a microwave plasma downdraft coal reactor using Ansys Fluent following an Eulerian–Lagrangian approach. Plasma conditions are taken from experimental data. The SIMPLE algorithm is used for velocity–pressure coupling and the $k-\epsilon$ model is used as the turbulence model. The results show an average temperature of 1350 K in the gasifier and a syngas with volume fractions of 18.4% of H₂ and 37.2% of CO. Ismail et al. [18,19,20] developed a homemade Euler–Euler model for plasma gasification. A parametric study was conducted to conclude that lower equivalence ratios favored H₂ and CO production, while higher ER values enhanced the carbon conversion efficiency (CCE). H₂ and CCE and cold-gas efficiency (CGE) were enhanced by higher steam-to-biomass ratios. For higher temperatures, H₂ and CO levels were improved as well as LHV, whereas CO₂ and CGE were reduced. They also found that higher plasma power is favorable to obtaining high-quality syngas but penalizes the process efficiency. Thus, this work is about to study the distribution of gas temperature and the mass fraction of the components of syngas in a updraft plasma reactor using computational fluid dynamics analysis in ANSYS Fluent in order to increment the limited knowledge existing in this area.

2. Materials and methods

2.1. Materials

The fuel used in the model was the Portuguese municipal solid waste (PMSW). According to Portuguese environment agency, the components of MSW are divided into its organic elements such as paper, degradable residues, textiles, composites, plastics, glass and metals. The organic materials of MSW were modeled to their basic elements (dry basis) and used as input material in the simulation. Table 1 presents the input characteristics the ultimate and proximate analysis of PMSW used in the theoretical study.

2.2. Methods

The model is developed based on a two-dimensional (2D) approach in Ansys Fluent of a updraft gasifier. Therefore, the symmetry conditions are used, which allows us to consider only half of the gasifier geometry shown

Table 1. Ultimate and proximate analysis of PMSW [21].

Proximate composition	Weight fraction (%)	Ultimate composition	Weight fraction (%)
Moisture	17.6	Carbon	48.0
Volatile matter	76.62	Hydrogen	6.3
Fixed carbon	8.46	Nitrogen	1.4
Ash	14.9	Oxygen	43.6

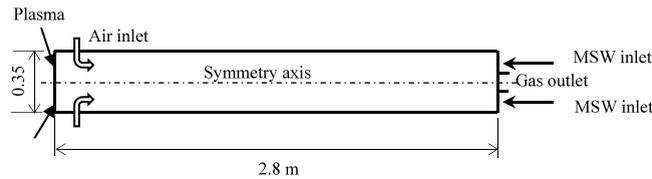


Fig. 1. Geometry of the updraft plasma gasifier.

in Fig. 1. The plasma is realized using the argon gas, which enters the gasifier at 1500 K. Air is used as the gasifying agent that enters the gasifier at 300 K. The produced gas leaves the top of the reactor through a central pipe with a diameter of 0.15 m. The MSW also enters through the top of the reactor but through a ring outside the produced gas pipe with a thickness of 0.10 m.

3. Mathematical model and numerical procedure

Computational fluid dynamics (CFD) is the science of predicting fluid flow, heat transfer, chemical reaction and other related phenomena by numerically solving a set of the governing mathematical equations mostly based on conservation equations of mass, energy, and momentum. However, due to the complexity of the plasma gasification process, involving various phases and many chemical and physical interactions among them not much works are available concerning the development of CFD models. Generally, results of CFD analysis are relevant for conceptual studies of new design, detailed product development, trouble shooting and redesign. Besides, CFD modeling is also cost-and-time-saving, safe and easy to scale-up [22]. Various numerical techniques have been employed in the solution of the CFD model’s equations. The most widely used numerical technique is the discretization method including the finite difference, finite element and finite volume methods. In the present work, a mathematical model is developed for simulating the flow inside an updraft plasma gasifier, considering continuity, species transport, heat transfer, turbulence and chemical reactions.

3.1. Mathematical model

The mass conservation equation or continuity equation is expressed as:

$$\frac{\partial \rho}{\partial t} + \nabla (\rho v) = S_m \tag{1}$$

where ρ is the local density, v is the fluid velocity, and the source term S_m represents the mass added to the fluid phase from the dispersed phase. Momentum equation is given as:

$$\frac{\partial \rho}{\partial t} + \nabla (\rho v v) = -\nabla p + \varphi g + F + \vec{\nabla} \vec{\tau} \tag{2}$$

where p is the static pressure, $\vec{\tau}$ is the stress tensor given by Eq. (3), and g , and F stand for the gravitational force and external body forces, respectively. The stress tensor $\vec{\tau}$ is defined as follows:

$$\vec{\tau} = \mu [\nabla v + \nabla v^t] - \frac{2}{3} \nabla v l \tag{3}$$

where μ is the molecular viscosity, v is the fluid velocity and l is the unit tensor. The standard k- ϵ model relies on solving the following two equations:

$$\frac{\partial}{\partial t} (\rho k) + \nabla (\rho u k) = \nabla \left(\frac{\mu_t}{\sigma_k} \nabla k \right) + G_k - \rho \epsilon \tag{4}$$

$$\frac{\partial}{\partial t} (\rho \varepsilon) + \nabla (\rho u \varepsilon) = \nabla \left(\frac{\mu_t}{\sigma_\varepsilon} \nabla \varepsilon \right) + C_{\varepsilon 1} G_k - C_{\varepsilon 2} \rho \varepsilon \quad (5)$$

where G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients and is expressed as follows:

$$G_k = \mu_t \nabla u [\nabla u + \nabla u^t] - \frac{2}{3} \nabla u (u_t \nabla u + \rho k) \quad (6)$$

$C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$, and the turbulent Prandtl numbers for k and ε are $\sigma_k = 1$ and $\sigma_\varepsilon = 1.33$, respectively [23]. The energy conservation equation is given by:

$$\frac{\partial \rho E}{\partial t} + \nabla (v (\rho E + p)) = \nabla \left(k_{eff} \nabla T - \sum_{\alpha=1}^N h_\alpha J_\alpha + \bar{\tau} v \right) + S_h \quad (7)$$

where the right-hand side of Eq. (7) includes energy transfer due to conduction, species diffusion, viscous dissipation, and heat of chemical reactions or other defined sources (S_h), respectively. k_{eff} is the effective heat conductivity equal to $k_{eff} = \omega + \omega'$, while ω' is the turbulent thermal conductivity defined according to the standard $k - \varepsilon$ model.

Species transport follows from species conservation equations, in which mass fraction y_α of the species α in the fluid phase satisfies the following convection–diffusion equation:

$$\frac{\partial (\rho y_\alpha)}{\partial t} + \nabla (v \rho y_\alpha) = \nabla J_\alpha + R_\alpha \quad (8)$$

where R_α is defined by:

$$R_\alpha = \begin{cases} -M_\alpha (v_{\alpha,1} R_1 + v_{\alpha,2} R_2) \\ M_\alpha (v_{\alpha,1} R_1 + v_{\alpha,2} R_2) \end{cases} \quad (9)$$

and the diffusion flux J_α is given as:

$$J_\alpha = -D_{t\alpha} \frac{\nabla T}{T} \begin{cases} \rho D_{m\alpha} \nabla y_\alpha \\ \rho (D_{m\alpha} + D_{t\alpha}) \nabla y_\alpha \end{cases} \quad (10)$$

Here, $D_{m\alpha}$ is the mass diffusion coefficient for the species α in the mixture, $D_{t\alpha}$ is the thermal (Soret) diffusion coefficient, and $D_{t\alpha}$ is the turbulent diffusivity defined as follows:

$$D_{t\alpha} = \frac{\mu_t}{\rho Sc_t} \quad (11)$$

In which μ_t is the turbulent viscosity and Sc_t is the turbulent Schmidt number (default value of 0.7). The trajectory of discrete phase particle follows from the equation:

$$\frac{d\mu_t}{dt} = F_D (v - u_p) + \frac{g(\rho - \rho_p)}{\rho_p} + F \quad (12)$$

where u_p denotes the particle velocity, v is the fluid phase velocity, F is the additional acceleration, and $F_D (v - u_p)$ is the drag force per unit of particle mass. F_D is defined by the following expression:

$$F_D = \frac{18\mu C_D Re}{24\rho_p d_p^2} \quad (13)$$

In which C_D is the dimensionless drag coefficient, ρ_p is the particle density and d_p is the instant particle diameter. Re is the relative Reynolds number. The most used overall simplified heterogeneous reactions are [24]:



Regarding the kinetic rate of reactions in the present model, data was obtained from [24,25]. Many factors influence the heterogeneous reactions, such as reactant diffusion, breaking up of char, and interaction with the

turbulent flow. In order to include both diffusion and kinetic effects, the Kinetic/Diffusion Surface Reaction Model was applied [26], where:

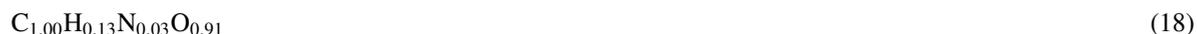
$$R_C = \frac{P_{O_2}}{K_r^{-1} + K_d^{-1}} \quad (15)$$

$$K_r = A_c T_s \exp\left(\frac{E_c}{RT_s}\right) \quad (16)$$

$$K_d = 5.06 \frac{10^{-7}}{d_p} \left(\frac{T_s + T_g}{2}\right)^{0.75} \quad (17)$$

where R_C is the char consumption rate, K_d is the diffusion rate and K_r is the kinetic rate. a_c is the pre-exponential factor equal to $3 \text{ kg m}^{-2} \text{ s}^{-2} \text{ Pa}^{-1} \text{ K}^{-1}$, and e_c is the activation energy.

Reaction models in this numerical simulation are adopted from ANSYS Fluent based on the following global chemical formula of PMSW:



The global chemical formula of the PMSW represents the ultimate analysis shown in Table 1. Because of the wide gap between the gas-phase and the solid particle reactions in terms of their kinetics, the finite rate/eddy dissipation is used to model the interaction between the chemical reactions and turbulence so that all the chemical reactions (chemically or eddy controlled) are accurately modeled.

3.2. Numerical procedure

In the current work, the previously described transport equations of mass, energy, momentum, and species are solved using the ANSYS Fluent program package. It uses the finite volume method for solving the equations resorting to the SIMPLE (semi-implicit method for pressure linked equations) algorithm [27]. This algorithm is essentially a guess-and correct procedure for the calculation of pressure and velocities on the staggered grid arrangement. The calculation sequence in a CFD procedure is given by an initial guess for pressure and velocities, resolution of the momentum equations, resolution of the pressure correction equation, pressure and velocities correction, and resolution of the all other transport equations.

Two assumptions were made for the realizable $k - \varepsilon$ model used for description of turbulence: the plasma flow is turbulent, and the effects of molecular viscosity are negligible. Radiation effects and magnetic field were neglected, and gravitational force is not included in the computations.

All boundary conditions of the computational domain were set according to known experimental values since major purpose of this model is to determine the distributions of physical properties and the distribution of mass fraction of the products of syngas. Heat losses to the reactor walls were always modeled by a prescribed heat flux. The inlet boundary of mass flow rate and temperature uses Dirichlet conditions, and the upper outlet boundary is set to pressure outlet. The wall surface applies no-slip condition.

For the species transport model, volume and particle surface reactions are selected, and the multi-step gasification reactions are calculated by the finite rate/eddy dissipation model.

4. Results and discussion

4.1. Model validation

The developed model results were compared with those found in Agon et al. [28] for refuse derived fuel at 1429 K, steam ratio of 1.6, and torch power of 120 kW in Fig. 2.

From the analysis of Fig. 2, it can be seen the good agreement of the model predictions with the experimental plasma gasification data. The relative error for the four main syngas species is below 12%, which can be considered a good performance of the developed model given the complexity of the plasma gasification process.

4.2. Temperature and gas species distributions

Fig. 3 shows the temperature profile along gasifier height. From the figure it may be seen that the combustion zone occurs at a temperature of 1500 K in the region of the plasma inlet. The identification of the combustion

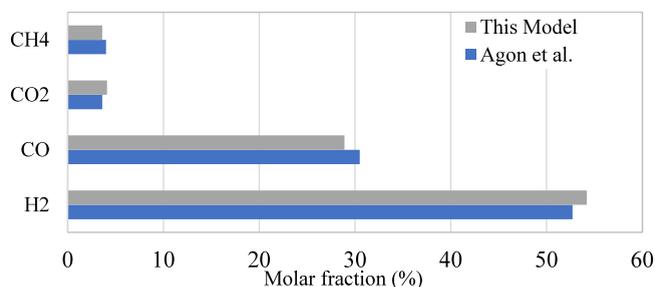


Fig. 2. Comparison between the present work and the results of Agon et al. [28].

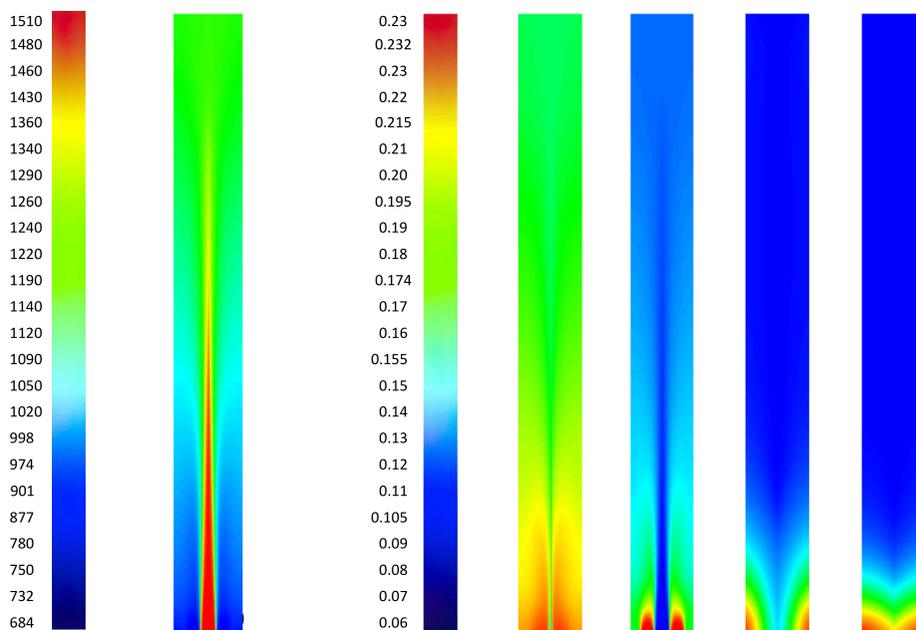


Fig. 3. Temperature and gas distribution fields under air plasma gasification.

zone is confirmed by the greater amounts of CO₂ in this region of the gasifier. The amount of heat released in the oxidation zone allows obtaining an average temperature in the reactor of around 1000 K, which agrees with the works of Ibrahimoglu et al. [17] and Zhang et al. [16].

The heat released in the combustion zone is used in the other gasification phases starting from the drying of the PMSW. After the evaporation of the PMSW moisture, the feedstock experiences decomposition in the so-called pyrolysis phase. The last phase of the gasification process occurs in the reduction zone. In this zone, most of combustible gases are produced. Therefore, the syngas quality depends on the extent of the reduction reactions, which in turn, are dependent on the gasifier temperature.

Fig. 3 also shows that the CO molar fraction is higher at the reactor bottom where a molar fraction of approximately 22% is reached. The CO formation is explained by two reactions: char combustion and pyrolysis. At the bottom of the reactor, higher temperatures enhance water-gas and Boudouard reactions, which contribute to the CO production. However, the molar fraction of CO decreases to about 17% at the gas outlet, which can be explained by the temperature difference due to combustion zone. CO moves upward and, in the middle of the reactor, reduction reactions take place such as water-gas-shift consuming CO and producing H₂.

The lower temperatures in the top of the reactor promote hydrogen production by the water-gas and steam methane reforming reactions. Hydrogen yield is very low (1%) at the reactor bottom, reaching a maximum of approximately 23% in the top of the reactor. Besides the water-gas-shift reaction, the increase in H₂ contents at high temperatures is also supported by the tar cracking and reforming reactions [29–32].

5. Conclusions

In this study, a numerical simulation of plasma gasification of municipal solid waste is done using species transport model to obtain the results of the molar fraction of produced gases within an air atmosphere and a plasma heat source. The SIMPLE algorithm is used in the numerical analyses for velocity–pressure coupling, and the $k - \epsilon$ turbulence model is chosen. The molar fraction of the produced syngas was compared with experimental results of the literature and found to be in good agreement.

The findings of this work show that the use of plasma greatly influence the quality of syngas. The temperature distribution showed that the updraft gasifier is actually operating at approximately 1000 K. It is well understood that increasing gasification temperature is beneficial since it enhances reaction rates, and alters the energy equilibrium of endothermic gasification. This emphasizes the importance of the current work because it depicts the various regions of the updraft reactor as well as the related gasification phases that occur in reality at different temperatures.

Despite its limitations, it is necessary to develop new designs and other ways for modeling the plasma gasification to optimize the interaction of a plasma flow with solid particles, liquids or other gases.

Modeling approach requires more research and development for wider and more reliable application of mathematical models for process optimization to enhance the understanding and the application of plasma gasification.

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.

Data availability

No data was used for the research described in the article.

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