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CFD Analysis of a Crucible Furnace Using Recycled PET as Fuel for Smelting Non-ferrous Metals

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The increasing accumulation of waste polyethylene terephthalate (PET) presents serious environmental problems, prompting the scientific community to develop waste management strategies. Despite the efforts, traditional mechanical recycling methods for PET face numerous limitations, leading to the exploration of alternative recycling approaches. Research has focused on exploring techniques such as PET combustion, but it has resulted in a complex process due to each plastics reacting differently when exposed to heat. A major advantage of quaternary recycling of PET is reducing the mass of solid by 70 % and can generate 475.73 kJ/kg of energy. This article presents a numerical study of a crucible furnace for non-ferrous metal smelting, fueled by methane-air and ground PET. The combustion is conducted under controlled conditions. A hydrodynamic analysis is performed by analyzing the pressure contours, velocity contours, and pathlines in the combustion chamber. A thermal and chemical study is also performed, analyzing temperature profiles and predicting flue gas emissions. The results show that the turbulence model used predicted eddy formation. The average temperature in the combustion chamber was 900 K, and species analysis at the furnace outlet indicates that this method is a sustainable and effective solution for waste plastic management.

1. Introduction

In Mexico, the estimated consumption of plastics is 66 kg/person/y, which 83 % ends up in open-air dumps (Secretary of the Environment, México 2023), while globally reported that 79 % of waste is buried in landfills. The most commonly used plastics are polypropylene (PP), polyethylene (PE), and polyethylene terephthalate (PET) (Matthews et al., 2021). These plastics are mostly single-use, and offer great versatility in applications due to excellent properties (Awaja and Pavel, 2005).

The PET food packing and beverage bottle and in textile fibers guarantees its dominance of this plastic in the global market (Joseph et al., 2024). PET packaging has many advantages over rigid packaging, both in its production and handling in transport of products, and it also allows food to be preserved in good condition (F.P.A., 2023). However, excessive consumption has led to PET waste representing 12 % of the world's plastic waste, approximately 70 M t/y (Babaremu et al., 2022). In the environment, PET has an intense resistance to bio-degradation due to its inert chemical stability (Zhao et al., 2017), which causes environmental risks when disposed of directly in landfills (Canopilo et al., 2020). Various measures have been adopted to combat this problem, such as reducing its use, reusing it, and recycling it.

At present, mechanical recycling remains the most widely used method for PET recycling, but it is limited when the waste PET is highly contaminated (Santomasi, 2024). Mechanical, biological, and chemical techniques have been developed for PET post-consumer recycling, but difficulties have been presented. For example, mechanical recycling causes PET thermomechanical degradation after several cycles of recycling. The incineration produces polycyclic aromatic hydrocarbons, polychlorinated biphenyls, heavy metals, toxic carbon,

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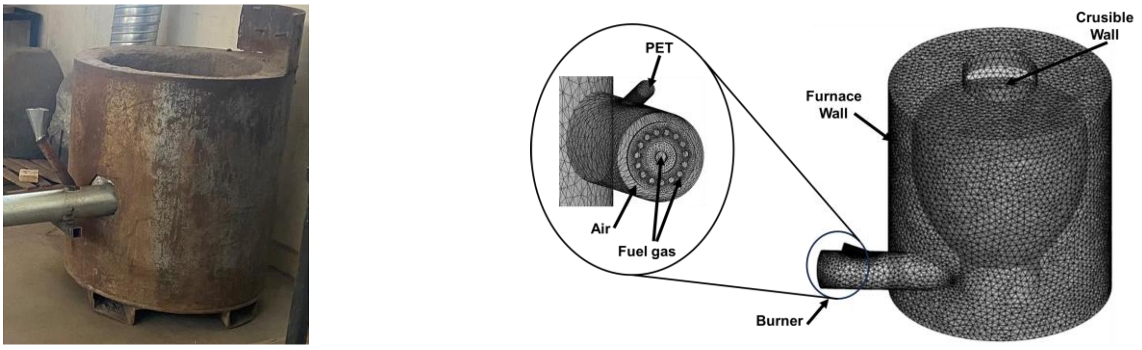
oxygen-based radicals, and greenhouse gases; hence this process is not considered a good alternative (Bharadwaj et al., 2024). Chemical recycling, glycolysis, biological recycling or biodegradation are expensive and time-consuming processes. (Bharadwaj et al., 2024). However, studies realized to PET combustion show in a controlled combustion, toxic products are generated a few quantities and reducing the solids waste by 70 % (Martín-Gullón et al., 2001). In addition, experimental and numerical studies of combustion have been conducted where generated energy is used (Filho et al., 2024). This energy is used in industrial processes that require heat energy, such as the cement industry and metal smelting. For this purpose, specialized equipment has been designed by CFD techniques (Cadavid et al., 2010). Liquid, solid and gaseous fuels combustion were modeled for different equipment (Zhang et al., 2019), besides radiation analysis realized (Xu et al., 2021) and toxic gases emissions for example NOx (Chang et al., 2021).

Previous research has involved experiments on mechanical recycling (Bezaraj et al., 2025), PET combustion in combination with other fuels (Hu et al., 2024), plastic mixtures combustion (Mentes et al., 2023) and pyrolysis (Song et al., 2023), which only focus on reducing solid waste in the environment. However, the calorific value that PET has for use as fuel is not used, which makes it attractive as an alternative energy source. This article presents the results of numerical simulation of the PET combustion process with energy recovery, applied in a crucible furnace using CFD. The CFD analysis allows for optimization of furnace design when using recycled PET as fuel. This analysis helps understand the thermal and fluid flow behavior within the furnace, leading to improvements in temperature distribution, combustion efficiency, and overall performance. The recovered energy generates heat that can be used to melt non-ferrous metals. The burner was designed for solids and adapted to the gas burner that supplies heat to the furnace. The analyses were conducted in transient state, using the k-epsilon model to model turbulent flows. The initial and boundary conditions were confidentially provided by a foundry company. Hydrodynamic, thermal, and chemical results were obtained, which were used to analyze the feasibility of PET as an environmentally friendly fuel. The results were compared with the Mexican Official Standard NOM-085-SEMARNAT-2011. The results presented are only numerical, as future work physical experiments will be conducted.

2. Mesh model and boundary conditions

A crucible furnace model was designed in CAD, which has 60 kg of aluminum capacity to melt up. The furnace is cylindrical, 0.73 m high, and 0.70 m in diameter. The crucible has a parabolic shape and is truncated at the base (diameter = 0.25 m) and the top (diameter = 0.53 m). The burner is located at the bottom and was adapted to feed PET fuel, see Figure 1a. Air and methane are fed into the burner, generating the flame and dragging the PET into the combustion chamber.



a) b)

Figure 1: a) Crucible furnace, b) Mesh and boundary condition of the crucible furnace.

The meshed model is shown in Figure 1b. The mesh is unstructured because the model presents irregular shapes throughout its domain. And this type of mesh allows its adaptation to the model. A total of 141,880 control volumes and 29,581 nodes were generated. Mesh sensitivity analysis was omitted for this work because there is evidence that it is impractical, according to Murrieta et al., (2019), since the study is performed without calculating the interface and in a transient state for 10 s.

Table 1 presents the boundary conditions used to perform the numerical simulations. The appropriate flow rate was determined based on experimental experience and stoichiometric calculations from a foundry company, and was provided confidentially for this work, allowing for safe investigation of combustion behavior. The crucible and furnace wall temperatures are considered constant (600 K), because the walls are considered adiabatic.

Table 1: Simulation data of combustion process.

Boundary condition type	Parameter	Value
Air inlet	inlet velocity	30 m/s
Methane gas inlet	inlet velocity	25 m/s
PET inlet	Mass Flow	0.1 kg/s
Furnace and crucible wall	Temperature	900 K
Gases outlet	Pressure outlet	1 atm
Time	Transient	10 s

3. Numerical Model

The PET combustion simulation process begins by solving the mass conservation equations, species, momentum, energy, ideal gas, and chemical kinetics reaction. The convective and diffusive terms are discretized using the second-order upwind and second-order central-difference schemes, respectively. Table 2 presents the spatial discretization schemes used in the simulation (ANSYS FLUENT, 2021).

Table 2: The spatial discretization schemes.

Variable	Discrete scheme
Pressure-velocity coupling	Coupled
Pressure	PRESTO
Density	Quick
Momentum	Second order upwind
Species	Second order upwind
Energy	Second order upwind

Turbulence was modeled using the k-epsilon standard. The Species Transport model was used for matter transport. The governing equations to coupled using the COUPLED model, and pressure was discretized using the PRESTO method. Simulations were performed considering only nine species, involving ten chemical reactions ($C_{10}H_8O_4$, O_2. C_4H_{10}, CO_2, H_2O, CH_4, C_2H_4, C_7H_8, CO, C_6H_6, H_2).

4. Results

4.1 Hydrodynamic behavior

3D modeling of combustion in a crucible furnace using CFD provides insight into the physical phenomena occurring in the reactor, which are not naturally easy to observe due to complexity of process. Figure 2a shows pathlines representing the movement of the fluid in the crucible. When the reactants are injected in the crucible, the gases have a horizontal linear movement, but the combustion reaction begins in this zone, which generates, heat energy and causes the expansion of gases, this phenomenon is known as cyclonic chamber. These results indicate that the k-e standard model adequately predicts fluid motion. Furthermore, due to the configuration of the furnace, the gases impact with the furnace refractory and the crucible wall; the flame cone flattens and elongates, wrapping a large part of the crucible surface, thus improving heat transfer. The Reynolds number for this flow is 54,000 approximately, which indicates the condition of turbulent flow. When the combustion gases turn around the crucible, they collide with the feed gases, causing heat gas eddies at the top and cold gas eddies at the bottom of the feed streamlines.

a)

b)

Figure 2: a) Pathlines of the flow, b) Pressure contours in the crucible furnace.

The inlet velocity is 30 m/s, but the gases expand inside the furnace, so the average velocity inside the furnace was 10.2 m/s. The gases generated by the combustion reaction have high temperatures, causing their density decrease and become lower than that of the outside air. The movement of the hot gases causes a pressure lower than atmospheric pressure. The total average pressure measured at time of 0.5 s is 200 Pa; this is represented by the red color (Figure 2b). The velocity contours were plotted, taking the shape of the flame cone (blue).

4.2 Thermal and chemical behavior

When the combustion reaction occurs, it releases heat energy, generating a long flat flame which rounds up the crucible. The highest temperatures are presented on the sides of the flame, where 1,200 K temperatures are predicted. However, the hottest fluid mixes with the low temperature gases, causing the dilution of the combustion gases, decreasing as well the average temperature in the combustion chamber to approximately 900 K. Fluid dilution is a consequence of the turbulent flow around the crucible. Figure 3 shows a temperature isosurface with a value of 900 K, which can be seen throughout the combustion chamber. The feed gases zone also is observed (green color).

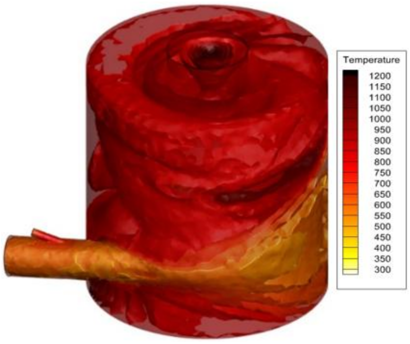


Figure 3: Temperature isosurface in the crucible furnace, 900 K.

Figure 4 shows a graph of time versus temperature, in which it can be observed that the temperature has quickly increased, because the temperature of the methane in the feed zone is 278.15 K, but when the combustion process begins, the temperature increases to 1,200 K. The end graph shows a rapid increase because at this point the oxidation reaction of all the reactants has already occurred. The temperature of the exhaust gases was measured at the furnace, averaging 857 K.

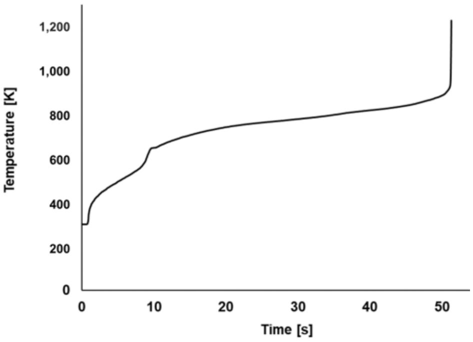


Figure 4: Graph of time [s] versus temperature [K].

PET combustion produces byproducts that come from undesired reactions that occur during the PET oxidation process. Combustion chemistry determines process efficiency, and both depend directly on the control of feed streams and process operating temperatures. Therefore, fuel is also required to generate the initial flame. This research work proposes PET combustion under controlled conditions, since previous studies (Guillon et al., 2001) reported that "clean combustion" is achieved at temperatures above 1,300 K. Considering PET ignition's point is at 900 K and in order to guarantee its combustion, furnace must to be preheated at 1,200 K.

The comparative graph of species formed by PET combustion in the simulation at the furnace outlet is presented in Figure 5. It can be observed that the gas present in the greatest quantity is CO, with a mass fraction of 5.9 X 10^{-4}, equivalent to 121 ppm. This result indicates that the furnace is operating within the parameters established by the Official Mexican Standard NOM-085-SEMARNAT-2011, which sets limits for this compound between 400 ppm and 500 ppm. The other gases are present in low quantities, for example, butane mass fractions are 1 X 10^{-4} and 2 X 10^{-4} for toluene.

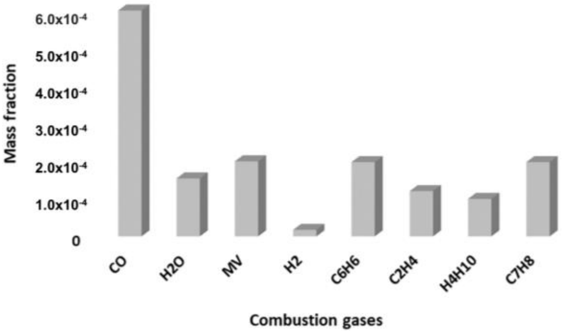


Figure 5: Comparative graph of mass fraction species.

Table 3 present the combustion reaction products measured at the furnace outlet. The measured volatile particles reached 57 ppm, which is below the standard value for solid combustion (60-350 ppm). Analysis of these data indicates that the amounts of reaction byproducts generated are present in lower quantities. Mentes et al. (2023) propose that aromatic compounds combust at temperatures of 1,100 K, and that at this temperature only CO_2 molecules are thermostable. Therefore, it is assumed that under the furnace operating conditions, PET combustion, can be considered "clean combustion", this contributes to reducing greenhouse gas emissions by utilizing plastic waste that would otherwise end up in landfills, as well as reducing natural gas consumption in the non-ferrous metal smelting process.

Table 3: Amounts of components in the furnace outlet.

Species	ppm
MV	57
CO_2	685
H_2O	31
H_2	3
CO	121
C_6H_6	53
C_4H_{10}	20
C_7H_8	40

5. Conclusions

In this research, a CFD analysis of PET combustion process applied for energy utilization was performed. The process was conducted in a model of a crucible furnace for the smelting of non-ferrous metals. Hydrodynamic, energy, and chemical reaction analyses were conducted in transient state.

The two-equation K-epsilon standard model which is useful to simulate swirl flows, presented excellent results in analyzing the flow inside the furnace. Eddies are generated within the furnace due to the collision of the stream and the chemical reaction of the feed fluids. The eddies formed in the upper part of the feed stream are the hottest gases, and those in the lower part are cold gases. The maximum velocity reached was determined to be 30.5 m/s, and the average velocity in the crucible was 10.2 m/s. The pressure was discretized using the PRESTO method, obtaining a pressure delta of 250 Pa.

The maximum temperature reached was 1,200 K in 5 s. The gas outlet temperature was measured at 857 K, and the average temperature inside the combustion chamber was 900 K, indicating that smelting of non-ferrous metals such as aluminum is feasible. Furthermore, combustion gas emissions were lower than those permitted by the Mexican Official Standard NOM-085-SEMARNAT-2011. According to these parameters, PET combustion under the conditions under in which this project was conducted can be considered "clean combustion."

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