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Simplified mathematical model of oxy-fuel combustion of municipal solid waste in the grate furnace: effect of different flue gas recirculation rates and comparison with conventional mode

Paulina Copik[a*], Andrzej Szlęk[a], Mario Ditaranto[b]

[a]Department of Thermal Technology, Silesian University of Technology, Konarskiego 22, Gliwice 44-100, Poland
[b]SINTEF Energy Research, Sem Sælands vei 11, 7034 Trondheim, Norway
*Corresponding author email: paulina.wienchol@polsl.pl

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Abstract

Bioenergy carbon capture technology (BioCCS or BECCS) plays a key role in the European Green Deal, which aims to decarbonize industry and energy sectors, resulting in the production of energy with negative CO_2 emissions. Due to the biogenic origin of carbon contained in municipal solid waste (MSW), the application of carbon capture in waste incineration plants can be classified as BioCCS. Thus, this technology has attracted scientists' attention recently since it reduces excessive waste and emissions of carbon dioxide. Currently, there are four incineration plants in the Netherlands, Norway and Japan, in which CO_2 capture is implemented; however, they are based on the post-combustion technique since it is the most mature method and not requires many changes in the system. Nevertheless, the separation of CO_2 from the flue gas flow, which contains mostly nitrogen, is complex and causes a large drop in the total performance of the system. Oxy-fuel combustion technology involves the replacement of air as an oxidizer into high purity oxygen and recirculated exhaust gas. As a result, CO_2-rich gas is produced that is practically ready for capture. The main goal of the study is to develop a mathematical model of oxy-waste combustion to answer the research questions, such as how the composition of oxidant that is supplied to the process affects the combustion performance. The model includes all important processes taking place within the chamber, such as pyrolysis, char burnout and gas combustion over the grate. The results of the work will contribute to the development of oxy-waste incineration plants and will be useful for design purposes.

Keywords: Oxy-fuel combustion; Mathematical modelling; Municipal solid waste; Carbon capture

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1. Introduction

Municipal solid waste (MSW) is recognised as an inevitable result of human activity, rapid urbanisation, and economic growth. By 2050, global waste production is expected to increase from 2.01 billion tonnes in 2016 to 3.40 billion tonnes [1]. The waste-to-energy (WtE) industry is of unquestionable significance for non-recyclable waste disposal and plays a key role in the waste management hierarchy established in the European Union (EU) Waste Framework Directive [2].

A grate furnace is a mature and reliable technique for waste

Nomenclature

$\bar{a}$ – Planck-mean absorption coefficient
A_i – pre-exponential factor or frequency factor, 1/s
c – specific heat capacity, J/(kg K)
E_i – energy activation, kJ/mol
H – enthalpy, kJ/kg
k – kinetic rate constant, 1/s
k_{diff} – coefficient of mass transfer
$\dot{m}$ – mass flow, kg/s
$\dot{Q}_{rad}$ – heat of radiation, kW
$\dot{Q}_{reac}$ – heat of reaction, kW
$\dot{Q}_{comb}$ – heat of combustion, kW
r – rate of reaction, kg/s
r_c – ratio of CO/CO_2 formation rate
R – universal gas constant, J/(mol K)
t – time, s
T – temperature, K
x – coordinate

Subscripts and Superscripts

bed – bed
dev – devolatilization
evp – evaporation
gas – surrounding gases
ox – oxidiser

Abbreviations and Acronyms

ASU – air separation unit
BECCS– bioenergy carbon capture and storage
CCS – carbon capture and storage
CHP – combined heat and power
GDP – gross domestic product
LCA – life cycle assessment
LHV – lower heating value
MEA – monoethanolamine
MSW – municipal solid waste
OFC – oxy-fuel combustion
TGA – thermogravimetric analysis
WtE – waste-to-energy

incineration that is also able to destroy and remove toxic organic substances [3]. As stated in [4], in the EU, the proportion of MSW incineration plants making use of moving grate technology is 88%.

A step forward in the development of WtE plants is the integration of incinerators with carbon capture and storage (CCS) technology to become carbon dioxide (CO_2) negative [5]. The described system is called bio-energy carbon capture technology (BioCCS or BECCS) and consists of CO_2 removal from the atmosphere through feedstock with biological origin, which is then thermally converted to obtain energy. The resulting biogenic carbon dioxide is captured and permanently stored, for instance, in a geologic formation, and the biomass is regrown [6].

The opportunities and challenges that need to be addressed to fully exploit the great potential of BECCS technologies based on MSW are summarised in our previous work [7], in which we concluded that among all CCS techniques, oxy-fuel combustion (OFC) is a promising technology in terms of energy efficiency and environmental impact. OFC involves increasing the partial pressure of carbon dioxide in the exhaust gases in order to facilitate and reduce the costs of its sequestration [8]. The schematic diagram of the oxy-MSW incineration plant is presented in Fig. 1. The process involves the employment of oxygen (O_2) instead of air as an oxidizer, resulting in a temperature increase. In the case of waste usually having a moderated or low calorific value, oxy-incineration is favourable since it reduces the consumption of auxiliary fossil fuels (it is often used to keep the required temperature in the MSW combustor, causing inevitable CO_2 emissions). Moreover, due to the absence of nitrogen (N_2), the volume of the flue gas stream is about 5 times lower, which facilitates the cleaning of flue gas and allows for reducing the size of equipment [9]. It can also be foreseen that an increase in the partial pressure of oxygen will intensify the oxidation of complex hydrocarbons. However, the issue with ash melting may occur due to the elevated temperature of the process. To control the temperature in the furnace, oxygen can be diluted with flue gas, which mainly consists of carbon dioxide and water vapour.

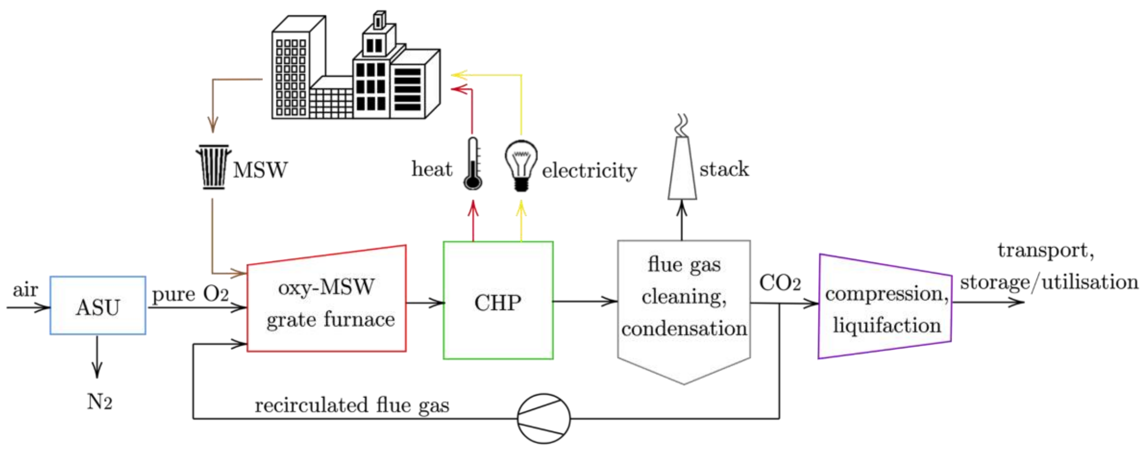


Fig. 1. Schematic diagram of the oxy-fuel incineration plant.

Till now, studies on oxy-waste combustion were focused on the assessment of the operation of the entire system, e.g. authors in [10–12] simulated the MSW incineration plant working under oxy-fuel combustion conditions and using exergy and life cycle assessment (LCA) analyses evaluated its exergy and energy efficiency as well as its effect on the environment. Results indicated that the total weighted resource consumption and total weighted environment potential of MSW oxy-fuel incineration were lower than MSW incineration with CO_2 capture via monoethanolamine (MEA) absorption. The authors also emphasized that the electric power consumption of the air separation unit (ASU) was the major influencing parameter, followed by the electric power consumption of the CO_2 compressor, while transport distance had a small influence on the results.

Experience from previous research on the oxy-combustion of fossil fuels, like coal, has shown that combustion chemistry and radiative heat transfer are altered due to the significantly higher partial pressures of carbon dioxide and water vapour in the flue gas [9,13–15]. Therefore, in the studies on oxy-waste combustion, the thermogravimetric technique was widely employed by many researchers to assess the thermal behaviour of waste, determine chemical kinetics and study gaseous emission in O_2/N_2 and O_2/CO_2 atmospheres [16–20]. Authors indicated that at the same oxygen concentration, the DTG (differential thermogravimetry) peak values in the oxy-fuel atmosphere were lower than those in the air atmosphere indicating that CO_2 has a higher inhibitory effect, as well as NO_x and SO_2 emissions were reduced at some temperatures under the O_2/CO_2 atmosphere. Thermogravimetric analysis (TGA) plays a vital role in research on the oxy-waste combustion process since it allows for relatively cost-effective and straightforward experimental data collection compared to tests using full-scale furnaces. As stated in [7], kinetic data obtained from TGA can be further used in mathematical and numerical modelling of the oxy-MSW combustion process.

In the literature, few works on the experimental investigation of oxy-waste combustion using lab-scale reactors can be also found, for example in [21,22]. Based on the results, authors concluded that such challenges as combustion chamber design, local O_2 concentrations, flue gas recirculation strategy as well as primary and secondary measures for NO_x should be further investigated. By now, only one study concerns an experimental campaign on OFC of wood chips using a pilot-scale facility [23]. The results of the tests indicated that the OFC of the biomass fuel is feasible but differs significantly from that of air combustion. The CO_2 concentration in the dry flue gas could be increased to around 73% with 5.7% excess O_2. Compared to air combustion, the emission of CO was higher during oxy-fired conditions, and the maximum temperature along the combustion chamber was lower.

Mathematical modelling is a powerful tool for furnace design and performance optimisation for various combustion systems without having to resort to scaling up results from lab-scale experiments, which is generally complicated by the strong interaction between turbulence, reaction kinetics, heat release and radiation. Research focused on the mathematical modelling of waste and biomass combustion on the grate furnace (Fig. 2) can be found in several papers, for example in [24–29]. Authors developed models of non-fossil solid fuel combustion with various levels of complexity that can be used for different purposes. All established models include processes such as drying, devolatilization, and gas and char oxidation, based on chemical kinetic to study different combustion indicators, e.g. temperature profiles, ignition and emission of pollutants. Since biomass and municipal solid waste contain high proportions of volatile matter, Yang et al. [30] built a one-dimensional model of solid fuel bed combustion to examine the effect of the devolatilization rate of the waste fuels on the process. In [31], authors developed a two-dimensional unsteady state model to investigate the effects of moisture content on combustion characteristics. Studies showed that due to the high moisture content of the feedstock, the evaporation process consumes a large amount of heat and can take about 2/3 of the whole combustion process. Research presented in [32] compared 2D and 3D models of waste combustion and investigated the effects of particle size, waste throughput, and residence time on the bed incineration performance. Yu et al. [33] developed a three-dimensional mathematical model as a tool for furnace structure design and operation conditions optimization when the straw combustion is in oxygen-enriched or air atmospheres. Such parameters as temperature and concentrations of carbon monoxide (CO) and nitrogen monoxide (NO) were calculated. The results of simulations showed that combustion in an oxygen-enriched atmosphere is superior to combustion in conventional air. A comprehensive review of modelling approaches of biomass and waste combustion is presented in [34] and [35], respectively.

Up to now, one paper on computational fluid dynamics (CFD) simulation of biomass thermal conversion under air/oxy-fuel conditions in a reciprocating grate boiler was found in the

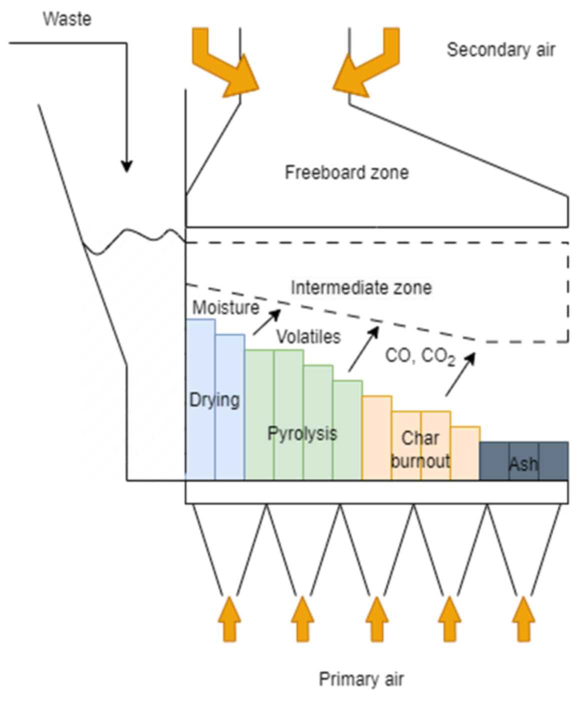


Fig. 2. Schematic diagram of the combustion chamber of a stoker boiler.

literature [36]. The effect of O_2/recycled flue gas (CO_2) ratios on flame temperature distribution, species concentration, char burnout, and fuel consumption have been studied and substantial differences were noticed compared with combustion in an air atmosphere. The numerical prediction showed that the gas temperature profile in oxy-fuel conditions with 25% oxygen concentration by volume in the oxidizer is closer to the referenced air-fired combustion.

To the best of the authors' knowledge, mathematical models of oxy-waste combustion in a moving grate furnace have not yet been described in the literature. Therefore, in this paper, a mathematical model of waste combustion for a full-scale moving grate MSWI plant under air- and oxy-fired conditions is demonstrated and compared. The model is developed using MATLAB Software. First, the air combustion model is validated by comparison with full-scale plant data. The validated model is then modified for an oxygen-fired system and used to study the effects of the atmosphere and oxidant distribution on important process outcomes.

2. Mathematical model development

2.1. Overview and assumptions

The scheme of considered MSW grate furnace is shown in Fig. 3. The combustion chamber is divided into three calculation sections: (a) grate, (b) intermediate zone, and (c) freeboard. In the model, the grate zone contains solid fuel particles. The oxidizer at the initial temperature and fresh fuel flow into the grate zone, where in the first stage the fuel is heated by surrounding gases by radiation, which provides energy for the evaporation and devolatilization. Then, the remained char reacts with oxidiser, which is supplied to the furnace, generating CO and CO_2. Therefore, fuel conversion processes take place in the grate zone, releasing or absorbing heat. This approach is consistent with most models of solid fuel combustion on the grate found in the literature [34,37]. The air in the grate zone is heated and partially consumed in the waste oxidation processes. The rest of the heated air and gases such as volatiles, water vapour, carbon dioxide and carbon monoxide escape from the grate zone. In the case of air combustion, the primary and secondary air is considered to be humid air. Temperature and relative humidity determine the absolute water content of air. For oxy-combustion, the oxidant is oxygen from the ASU and recycled exhaust gases. The composition of the oxidant that was adopted during the simulations is given in Table 2.

As Hoang et al. [35] stated, the coupling between the waste bed and the freeboard is a concern during mathematical modelling. Therefore, in this study, the intermediate zone is proposed, in which the released combustible gases like carbon monoxide and volatile matter are partially combusted with the surplus oxidizer from the grate zone; thus, heat is released above the grate. The reactions follow a chemical equilibrium. Such a solution has not yet been found in the literature.

In the freeboard, the oxidiser is supplied again to ensure the complete combustion of remaining combustible gases. The produced flue gas contains mainly CO_2, H_2O, and excess O_2. Thus, after water condensation, CO_2 can be easily compressed and transported.

The main assumptions are as follows:

- Waste is described by proximate and ultimate analysis.
- Model is steady state.

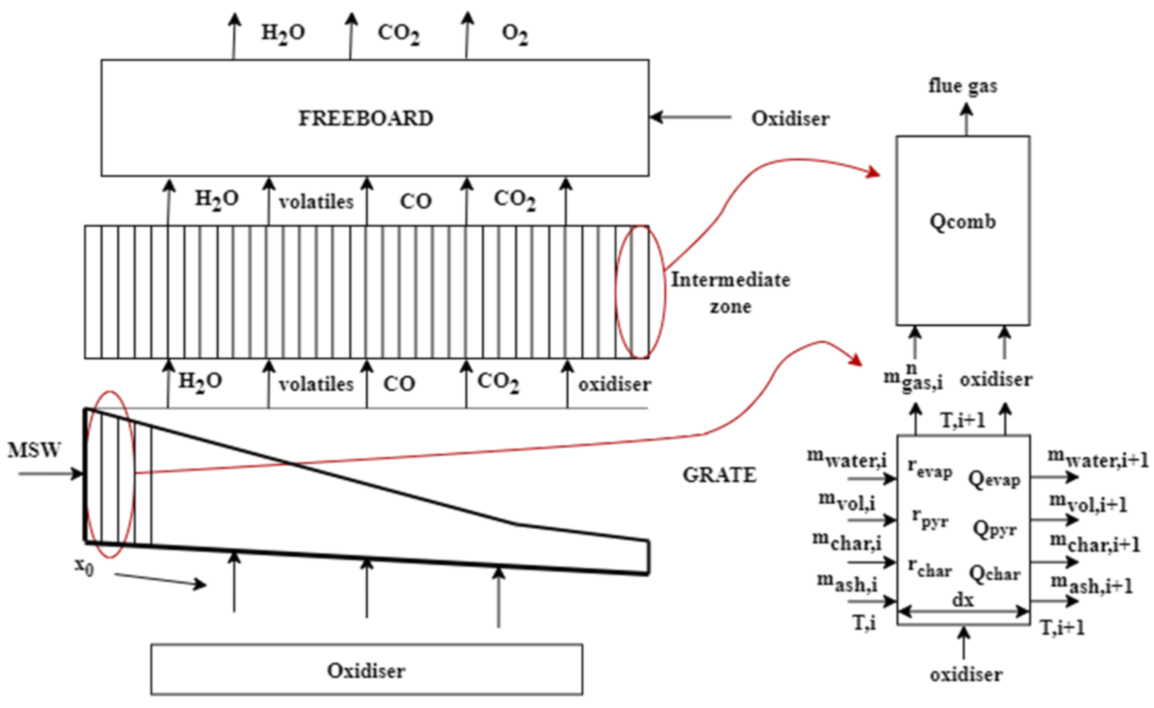


Fig. 3. Model of MSW combustion chamber.

- The modelled grate and intermediate zones are one-dimensional; the freeboard is modelled as 0D.
- Grate and intermediate zones are discretized in the direction of the moving grate as a series of control volumes. State variables within each control volume are homogeneous.
- Pyrolysis and char burnout that take place on the grate are taken into account based on one-step chemical kinetics.
- Combustion of volatiles and gases produced during char burnout that takes place over the grate is complete.

2.2. Materials

Municipal solid waste is a mixture of paper, plastic, food, textiles, tyres/rubber, glass and others. Determining the physicochemical properties of municipal solid waste is often problematic due to the high variability and heterogeneity of the feedstock [38]. The composition of waste varies depending on the level of gross domestic product (GDP) and the lifestyle of society, but may also vary depending on the season [7]. However, it can be assumed that the general properties of Europe's MSW are as follows: a) relatively high moisture content of 10–20%, b) high volatiles (VM) content at about 60–80% (dry basis), c) the ash fraction exceeding 10%, and d) fixed carbon (FC) level of about 10–20%. The average ultimate MSW composition can also be proposed (daf basis): 40–50% C; 25–35% O; 5–7% H; 0.5–2% N; 0.1–0.2% S; 0.1–0.2% Cl with a moisture content of 20–40% and an ash content of 15–30% [39].

In this study, we took the properties of waste, such as spent coffee grounds, described in detail in our previous study on kinetic analysis [20], but because the tested materials were dry, the amount of moisture was adjusted to match waste that is typically combusted in waste incineration plants. The proximate and ultimate analyses are presented in Table 1.

Table 1. Fuel composition.

Proximate analysis					
Moisture (ar, wt%)	Volatile matter (db, wt%)		Fixed carbon (db, wt%)		Ash (db, wt%)
20	57.77		7.62		34.61
Ultimate analysis (dry basis, wt%)					
LHV, kJ/kg	C	H	O	N	S
14 784	43.50	5.50	15.28	0.13	0.01

2.3. Mass and energy balances

The mass flow loss in each control volume is calculated as follows:

$$\frac{d\dot{m}_{tot,i}}{dx} = -k_j dt \dot{m}_{tot,i}, \tag{1}$$

where $d\dot{m}_{tot,i}$ is the mass flow loss of the fuel (kg/s), dx is the length of the control volume (m); k_j is the rate of the jth process (drying, pyrolysis, char burnout) (1/s); dt is the fuel residence time (s); described as

$$dt = \frac{dx}{v}, \tag{2}$$

where v is grate velocity (m/s).

The energy balance for the municipal solid waste bed is modelled as

$$\frac{\dot{m}_{tot,i} c_{tot,i} dT_i}{dx} = \dot{H}_{bed,i} - \dot{H}_{bed,i+1} + \dot{Q}_{rad,i} + \dot{H}_{ox,i}^{in,grate} - \dot{H}_{ox,i+1}^{out,grate} + \dot{Q}_{reac,i} - \dot{H}_{gas,i+1}^{out,grate}, \tag{2}$$

where $\dot{Q}_{rad,i}$ is the heat of radiation (kW/m), $\dot{H}_{ox,i}^{in,grate}$ and $\dot{H}_{ox,i+1}^{out,grate}$ denote the enthalpy flux of the oxidant at the inlet and outlet of the ith control volume (kW/m), respectively, $\dot{Q}_{reac,i}$ is the heat of the reactions (evaporation, pyrolysis, char oxidation) in the ith control volume (kW/m), $\dot{H}_{bed,i}$ and $\dot{H}_{bed,i+1}$ are the physical enthalpy fluxes of the solid bed at the inlet and outlet of the ith control volume (kW/m), respectively, $\dot{H}_{gas,i+1}^{out,grate}$ is the physical enthalpy of the gaseous phase escaping from the ith control volume (kW/m), and $\dot{m}_{tot,i}$ is defined as

$$\dot{m}_{tot,i} = \dot{m}_{water,i} + \dot{m}_{waste,i} + \dot{m}_{char,i} + \dot{m}_{ash,i}, \tag{4}$$

where $\dot{m}_{water,i}$, $\dot{m}_{waste,i}$, $\dot{m}_{char,i}$ and $\dot{m}_{ash,i}$ are the mass flow of the water, dry waste, char and ash in the solid bed, respectively. Parameters $c_{tot,i}$ (J/(kg K)) and T_i (K) denote specific heat capacity and temperature in the ith control volume, respectively.

2.3.1. Moisture evaporation zone

The rate of moisture release from solids can be expressed as [27,28,40]

$$r_{evp} = A_s h_s (C_{w,s} - C_{w,g}) \quad \text{when} \quad T_s < 100\,°\text{C} \tag{5}$$

or

$$r_{evp} = \frac{\dot{Q}_{rad}}{H_{evp}} \quad \text{when} \quad T_s \geq 100\,°\text{C}, \tag{6}$$

where H_{evp} is the heat of vaporisation of moisture contained in the solid (kJ/kg), h_s is the convective mass transfer coefficient (m/s), calculated according to [34], $C_{w,s}$ and $C_{w,g}$ is the moisture concentration in the solid phase and gas phase, respectively (kg/m^3), A_s is particle surface area (m^2), and Q_{rad} is radiation heat transfer (kW), and T_s is the temperature of the solid (°C).

2.3.2. Devolatilization zone

Pyrolysis is a crucial stage of combustion, where volatile compounds are released and the char is formed. Due to the complexity of the pyrolysis process, in this study, the devolatilization of waste is described by a one-step global reaction:

$$\text{MSW} \xrightarrow{r_{dev}} \text{char} + \text{volatiles}. \tag{7}$$

The rate constant of volatile release is taken from an Arrhenius type of expression:

$$k_{dev} = A_1 \exp\left(\frac{-E_1}{RT_{grate}}\right), \tag{8}$$

where A_1 is the pre-exponential factor or the frequency factor (1/s), E_1 is the energy activation (kJ/mol), and R is the universal gas constant (J/(mol K)). The data used for the calculation are presented in Table 3.

2.3.3 Char burnout zone

Due to the reactivity of CO_2 diluent, char combustion is influenced by various mechanisms, such as reduced oxygen mass transfer in CO_2, the lower temperature due to the higher heat capacity of CO_2 and the char-CO_2 gasification reactions [41]. In this study, the oxidizing (exothermic) reaction of char with oxygen is considered, in which CO_2 and CO are produced:

$$\mathrm{C} + \frac{1}{\theta}\mathrm{O_2} \xrightarrow{r_2} 2\left(1-\frac{1}{\theta}\right)\mathrm{CO} + \left(\frac{2}{\theta}-1\right)\mathrm{CO_2}, \tag{9}$$

where θ is the stoichiometric ratio for char oxidation defined as

$$\theta = \frac{1+\frac{1}{r_c}}{\frac{1}{2}+\frac{1}{r_c}}, \tag{10}$$

where r_c is the ratio of CO/CO_2 formation rate, which can be estimated by

$$r_c = \frac{\mathrm{CO}}{\mathrm{CO_2}} = 12\exp\left(-\frac{3300}{T_{char}}\right), \tag{11}$$

where T_{char} represents the char temperature.

The char reaction rate that can be generally expressed as [42]

$$k_i = \frac{k_{kin,i}k_{diff,i}}{k_{kin,i}+k_{diff,i}}, \tag{12}$$

where $k_{diff,i}$ is the coefficient of mass transfer for oxidizing and reductive reaction (kg/(m^{2}sPa), and

$$k_{kin,i} = A_i \exp\left[\frac{-E_i}{RT_{char}}\right] \tag{13}$$

is the kinetic rate constant for oxidizing and reductive reaction (kg/(m^{2}sPa)).

2.3.4. Intermediate zone – gaseous phase partial combustion

The energy balance of the intermediate zone is calculated as follows:

$$\frac{\dot{m}_{gas,i}c_{gas,i}dT_i}{dx} = \dot{H}_{ox,i}^{out,grate} + \dot{H}_{gas,i}^{out,grate} + \dot{Q}_{comb,i} - \dot{H}_{gas,i}^{out,intermediate\ zone}, \tag{14}$$

where $c_{gas,i}$ stands for the specific heat capacity of the gas produced in the ith control volume (J/(kg K)), $\dot{Q}_{comb,i}$ is the heat of partial combustion of volatiles and combustible gases (kW/m), $\dot{H}_{gas,i}^{out,intermediate\ zone}$ is the enthalpy of the produced gas at the outlet of the ith control volume (kW/m).

2.4. Heat transfer between solid and gaseous phases

Since high temperature occurs in the combustion chamber, this model assumes that radiation is the dominant heat transfer mechanism:

$$\dot{Q}_{rad,i} = \frac{\varepsilon_{bed}+1}{2}A\sigma\left(\varepsilon_{gas}T_{gas}^4 - \sigma_{gas}T_{bed}^4\right). \tag{15}$$

The emissivity ε_{bed} depends on the material, temperature and surface condition. In our simulations, we used a constant emissivity of ε_{bed} = 0.8 for waste bed, but different emissivities can be used for different fractions if data are available. In the above, A denotes surface (m^2), T_{gas} is the temperature of the freeboard (K), T_{bed} is the temperature of the grate (K), and σ is the Stefan-Boltzmann constant, $\sigma = 5.67\times10^{-8}$ W/(m^{2}K^4).

To calculate the radiative properties of gases in the furnace (ε_{gas} and α_{gas}), the weighted sum of the grey gases model (WSGGM) is used, which was introduced by Hottel and Sarofim [43] and due to its simplicity and relatively high accuracy, it was further developed and used by many researchers [38,44].

In the WSGG model, the Planck-mean absorption coefficient of the gas mixture over a path length is determined by [41,45]

$$\bar{a} = -\ln(1-\varepsilon/s), \tag{16}$$

where s is the radiation beam length, and ε the gas emissivity. The latter is calculated from

$$\varepsilon = \textstyle\sum_i a_{\varepsilon,i}(T)(1-\exp(-\kappa_i p_i s)), \tag{17}$$

where $a_{\varepsilon,i}$ is the emissivity weighting factor for the ith grey gas component, κ_i and p_i are the pressure absorption coefficient (1/m·atm) and partial pressure (atm) of the ith absorbing gas, respectively.

The emissivity weighting factors are polynomial correlations that can be given as a function of the gas temperature:

$$a_{\varepsilon,i} = \textstyle\sum_j b_{\varepsilon,i,j}T^{j-1}. \tag{18}$$

It should be noted that most of the already established coefficients of WSGGM are suitable only for the air-fired combustion conditions, where the molar fractions ratio of carbon dioxide and water vapour differs from oxy-fuel combustion, and using them in the oxy-fired conditions may lead to uncertain levels of inaccuracy. Therefore, with the growing popularity of oxygen-fired systems, some scientists have expanded the set of coefficients with those dedicated to oxy-fuel combustion, for example, in [45,46].

3. Calculation data

Physical data and process data (Table 2) of the full-scale incineration plant were provided by the Returkraft WtE plant in Kris-

Table 2. Physical and process data.

Parameter	Unit	Value
Grate length	m	10.2
Grate width	m	6.3
Height to the top of 1st pass	m	19.15
Waste throughput capacity	t/h	18
Primary air distribution (5 zones) (air-fired mode)	%	8 – 29 – 37 – 23 – 3
Primary air temperature	°C	110
Primary air flow rate	m_n^3/h	53669
Secondary air temperature	°C	110
Secondary air flow rate	m_n^3/h	39945
Grate speed	m/s	0.002
Oxidiser composition (air-fired mode)	vol. %	21% O_2 – 79% N_2
Relative humidity	%	95
Oxidiser composition (oxy-fired mode)	vol. %	95% O_2 – 5% N_2
Wet recirculated flue gas composition (oxy-fired mode)	mol %	55.5% CO_2 – 27.7% H_2O – 12.2% O_2 - 4.4% N_2
Flue gas molar flow	kmol/s	0.9429

tiansand (Norway). A description of the waste incineration process at the studied plant is available in [38].

As mentioned earlier, in this study individual steps of the fuel thermal decomposition were taken into account based on chemical kinetics. To determine the kinetic parameters of waste materials, an experimental campaign on the thermogravimetric instrument and lab-scale reactor was performed. Firstly, we performed the TGA analysis of sample pyrolysis in N_2 and CO_2 atmospheres and retrieved the kinetic data, employing isoconversional methods, also known as model-free (Friedman and Vyazovkin). According to the isoconversional principle, the process rate at a constant extent of conversion α is a function of temperature [47]. Then, we used a lab-scale reactor to produce waste chars and we subjected them to thermogravimetric analysis in air and oxy-fired conditions. These studies were in detail described in our previous works [20,21]. Table 3 shows the kinetic data used in the mathematical model in the air- and oxy-fired modes.

Other calculation data, such as, the physical properties of used waste used in the model are summarized in Table 4.

For the simulation of the waste combustion system, MATLAB software was used. The equations were solved using Newton-Raphson method and a mesh array of 10200 was employed.

4. Results and discussion

In the study, firstly simulations of the incineration chamber in the air-fired mode were performed, using assumptions and equations presented in Section 2 and input data presented in Section 3. The results of these calculations, such as the temperature of the grate and intermediate zone, as well as the mass flow of waste as a function of grate length, together with the model verification, are provided as a 'reference' and presented in Section 4.1. Validated model was then modified to the oxy-fired mode using the input data from Section 3. The results of the analysis of oxy-fired system are presented in Section 4.2.

4.1. Reference simulation and comparison with process data

Figure 4a presents the temperature of the grate and intermediate zone, as well as the fuel mass flow as a function of grate length. As can be observed, fuel combustion on the grate occurs gradually. Firstly, the fuel heats up and dries (Zone I), then when the grate reaches a temperature of around 450°C, volatiles are released. The drying and pyrolysis processes end at a distance of 2 m of the grate. Directly above the grate, in the intermediate zone, the volatiles partially burn, releasing heat and causing temperature growth up to 2000 K (Zone II). After the pyrolysis process, the waste char begins to slowly oxidize, and over the grate length of 8 m the fuel is burned out (Zones III and IV). In the fifth zone, the air mass flow is reduced and only ash remains. Similar findings regarding weight loss on the grate, burnout and grate temperatures have been found in the literature [27,28,30,38]. The different zones shown in Fig. 4a correspond to the air distribution according to data obtained from an incinerator in Norway (Table 2).

Figure 4b presents the molar fractions of gas species in the intermediate zone. As can be seen, oxygen quickly drops from 21% to below 1%, meaning that it is consumed during most of the process on the grate, which indicates that locally the air-lean (or fuel-rich) conditions dominate the bed combustion processes [33]. After the complete combustion of the fuel, the intermediate

Table 3. Kinetic data used in the mathematical model in the air- and oxy-fired mode.

Parameter	Unit	Value
$A_{dev,air}$	1/s	$10^{17.7}$
$E_{dev,air}$	kJ/mol	232100
$A_{dev,oxy}$	1/s	$10^{21.3}$
$E_{dev,oxy}$	kJ/mol	274700
$A_{char,air}$	1/s	$10^{4.79}$
$E_{char,air}$	kJ/mol	104372
$A_{char,oxy}$	1/s	136.56
$E_{char,oxy}$	kJ/mol	72137

Table 4. Physical properties of waste used in the model [24,27,29].

Parameter	Unit	Value
Heat capacity of water, c_{water}	kJ/kgK	4.187
Heat capacity of dry waste, c_{waste}	kJ/kgK	1.5+0.001T
Heat capacity of char, c_{char}	kJ/kgK	0.44+0.001T $^{-7}$×10^{-8} T^2
Heat capacity of ash, c_{ash}	kJ/kgK	0.8
Bed emissivity, ε_{bed}	–	0.8
Gas emissivity (air-fired system), $\varepsilon_{gas,air}$	–	0.4143
Gas emissivity (oxy-fired system), $\varepsilon_{gas,oxy}$	–	0.4816

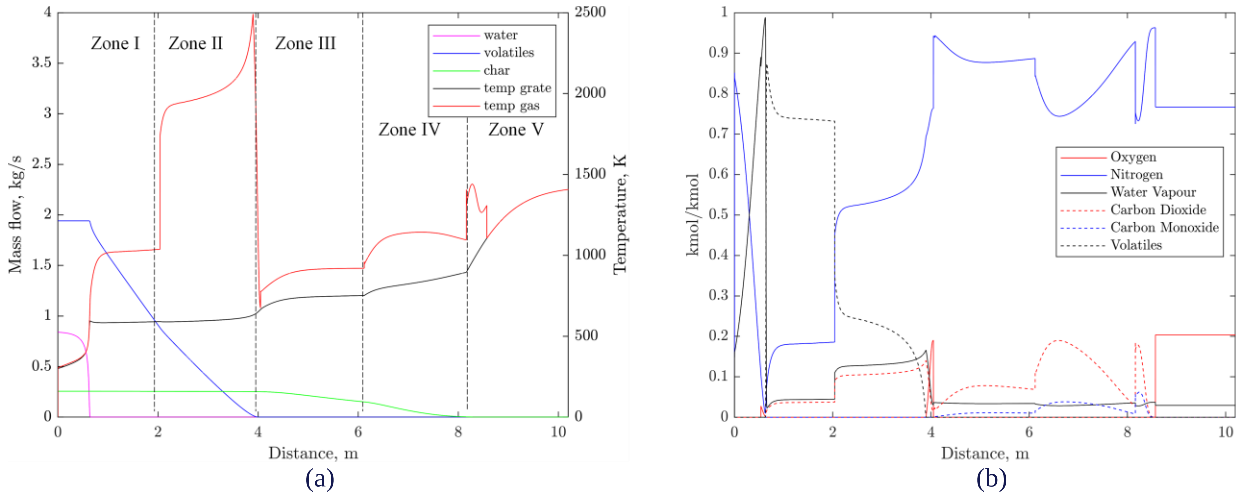


Fig. 4.(a) Temperature of the grate and intermediate zone and the mass flow of the fuel as a function of grate length; (b) Molar fractions of gas species in the intermediate zone.

zone is filled only with air. Results indicate that during the char oxidation CO_2 generation is more intensive. The produced carbon monoxide will be further combusted in the intermediate zone above the grate generating heat. Nevertheless, it is worth mentioning that in the char burnout zone, the temperature should not exceed 800°C due to the presence of organics in the waste, such as plant residues and food leftovers with a very low ash melting point temperature of around 825°C [48].

Figure 5 presents a comparison of the temperature of the

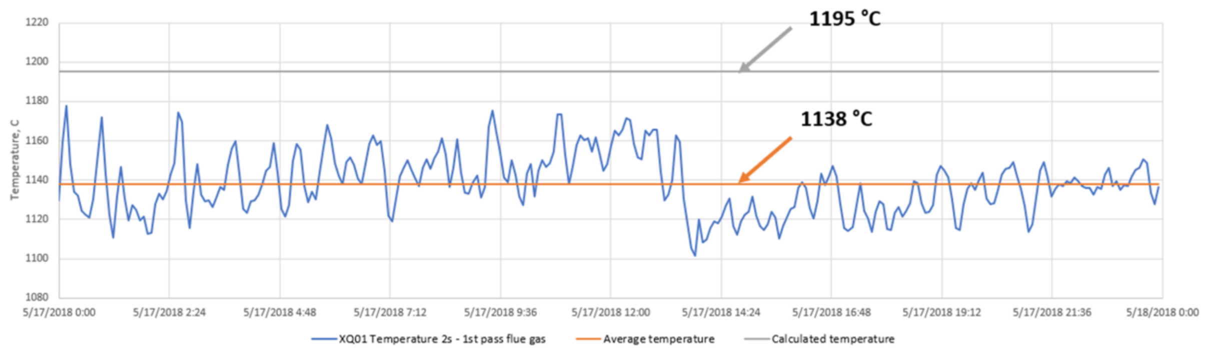


Fig. 5. Comparison between real temperature in the furnace (freeboard zone) and simulation results (WtE Returkraft plant data).

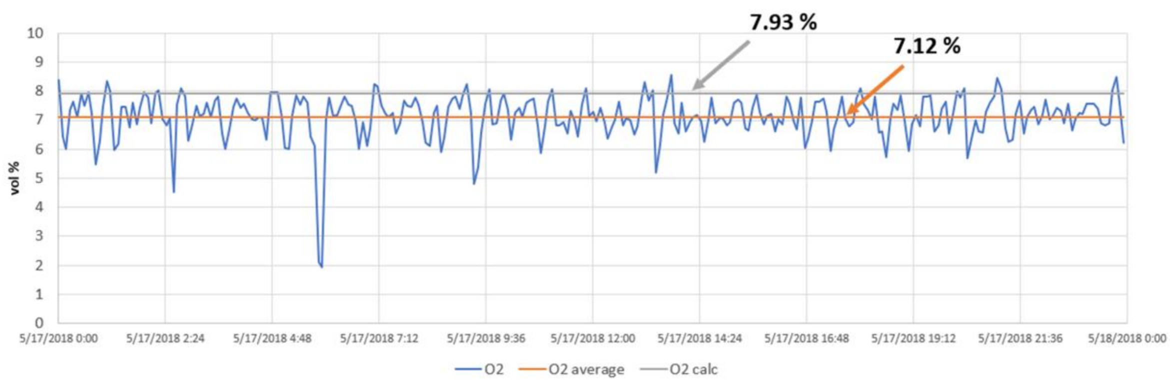


Fig. 6. Comparison between the measured and simulated oxygen content in the flue gas at the outlet (WtE Returkraft plant data).

freeboard between the air-fired model and the measurements (with the calculated average value) in the incineration plant. Figure 6 shows measurements and the calculated value of the oxygen content in the flue gas at the outlet. The relative difference between the calculated and measured values of temperatures and oxygen content is 4.8% and 10.2%, respectively. Thus, it was found that the air-fired model was sufficiently accurate and work on the model in the oxy-combustion mode began.

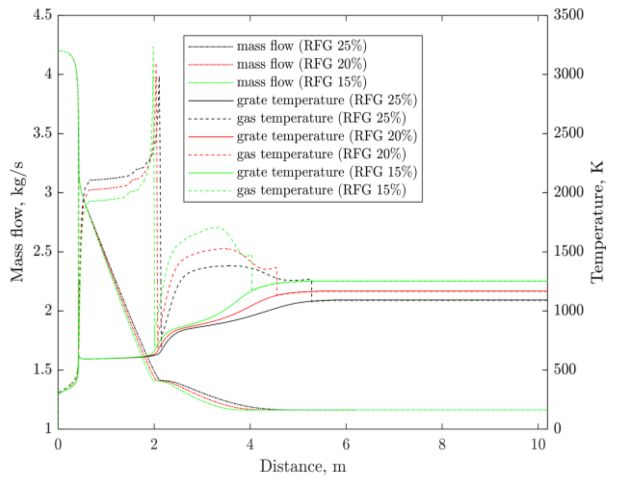
4.2. Oxy-combustion model

This section presents the results of simulations of the oxy-waste combustion chamber. To assess the influence of different factors, such as flue gas recirculation ratio, oxygen distribution, and oxidizer temperature, three different cases were studied:

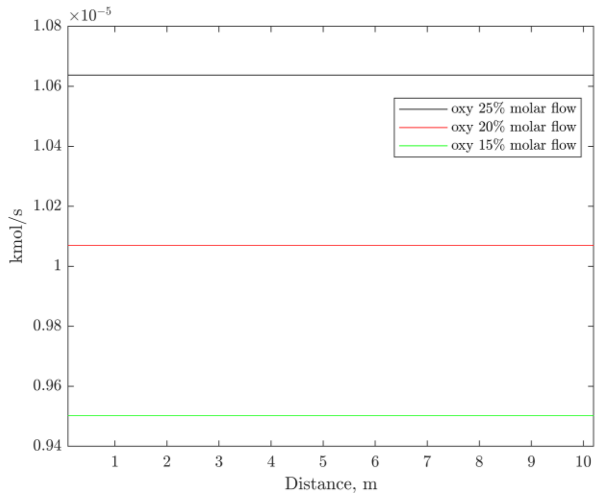
1) The first one involved introducing oxygen into the combustion chamber in a sub-stoichiometric amount (λ equal to 0.52), along with recirculated exhaust gas in the ratio of 15, 20, and 25%.
2) The second one comprised checking the influence of oxidant distribution. This was achieved by first supplying recirculated flue gas to the combustion chamber, and only after the volatiles have been released, introducing oxygen (in the amount as in the first case).
3) In the third case, the most favourable oxygen distribution was taken (determined from the previous cases) and the influence of 3 different oxidant temperatures on the process was checked.

4.2.1. Effect of the flue gas recirculation

Oxy-fuel combustion changes many parameters inside the furnace due to the change in overall thermal environment in the furnace. A major effect is visible on temperature distribution which happens due to CO_2 rich combustion environment. Figure 7 presents the radiative heat transfer between gas and solid phase for air- and oxy-fired conditions. As can be observed, oxy-fired system is characterized by higher radiative heat flux than combustion in an air atmosphere, which can be also observed in other comparative studies on air- and oxy-fired systems [41,49].



(a)



(b)

Fig. 8. a) Temperature of the grate and intermediate zone, and the mass flow of the fuel as a function of grate length; b) Oxidant distribution along the grate.

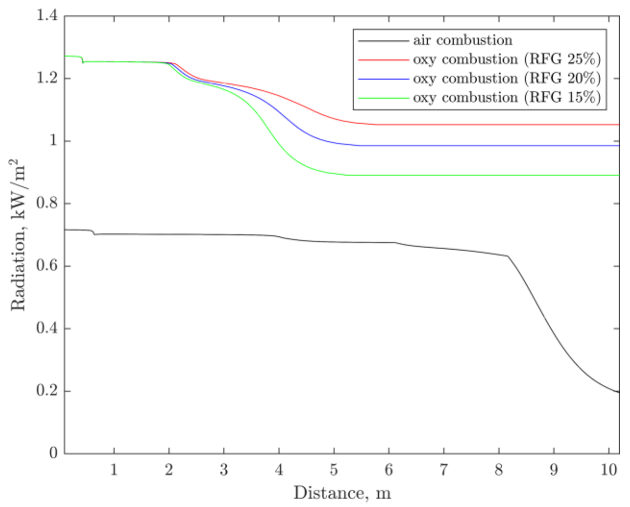


Fig. 7. Radiative heat transfer for air- and oxy-fired system.

Figure 8 shows temperatures of the grate and intermediate zone, as well as the mass flow of waste as a function of grate length. As can be observed, the higher the degree of flue gas recirculation, the lower the temperature of the grate and the intermediate zone, which confirms that recirculation can effectively control the temperature in the combustion chamber. The reason for this is the change in the environment of the furnace, as the CO_2 and H_2O contained in flue gas have a different specific heat capacity than N_2. The increased amount of recycled flue gas decreases the temperature of the process [36,50].

The next finding obtained in this research is that using oxygen during waste combustion raises the temperature and speeds up the process. For instance, combustion ends at 4 m for a recirculation rate of 15%, at 4.5 m for a 20% rate, and at 5.5 m for

Table 5. Oxygen demand for different oxy-fired conditions.

Parameter	Unit	Value		
RFG ratio	%	15	20	25
Total oxygen demand	kmol/s	0.0969	0.1027	0.1085
Oxygen from ASU	kmol/s	0.0795		
Share of oxygen in the oxidant	%	33	37	43

25%. This means that, in addition to the lower exhaust gas volume and thus, smaller equipment used for flue gas cleaning (as discussed in Section 1), the size of the combustion chambers operating under oxy-fuel conditions may be lowered by 30–50% when compared to the conventional mode of combustion.

The oxygen needed to complete the oxy-waste combustion process (total and oxygen produced in ASU) is compiled in Table 5. A larger flue gas recirculation (RFG) ratio corresponds with a higher oxygen content in the oxidiser. This is because components that oxidize, like oxygen, carbon dioxide, and water vapour, are present in the recirculated gases. Additionally, the percentage of oxygen in the oxidant was determined for each case and ranged from 33% to 43%.

Nevertheless, we found that temperature in the intermediate zone can exceed as much as 3000 K, when the volatiles are partially combusted, and the temperature at the grate can exceed the temperature of the waste ash melting point. Thus we analysed the second case, in which we limited the oxygen supply only to char oxidation zone. The drying and devolatilization processes were carried out in the atmosphere of recycled flue gases (with ratios of 15, 20 and 25%).

4.2.2. Effect of oxygen distribution

Analogous to the previous results, Fig. 9 shows a comparison of radiative heat transfer between air- and oxy-fired conditions for different ratios of flue gas recirculation. The oxygen share in the oxidant for each case was equal to 25%. It can be observed that

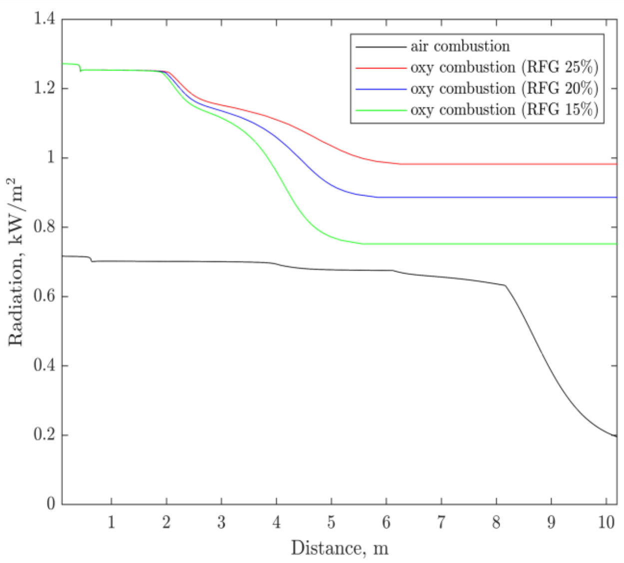


Fig. 9. Radiative heat transfer for air- and oxy-fired system.

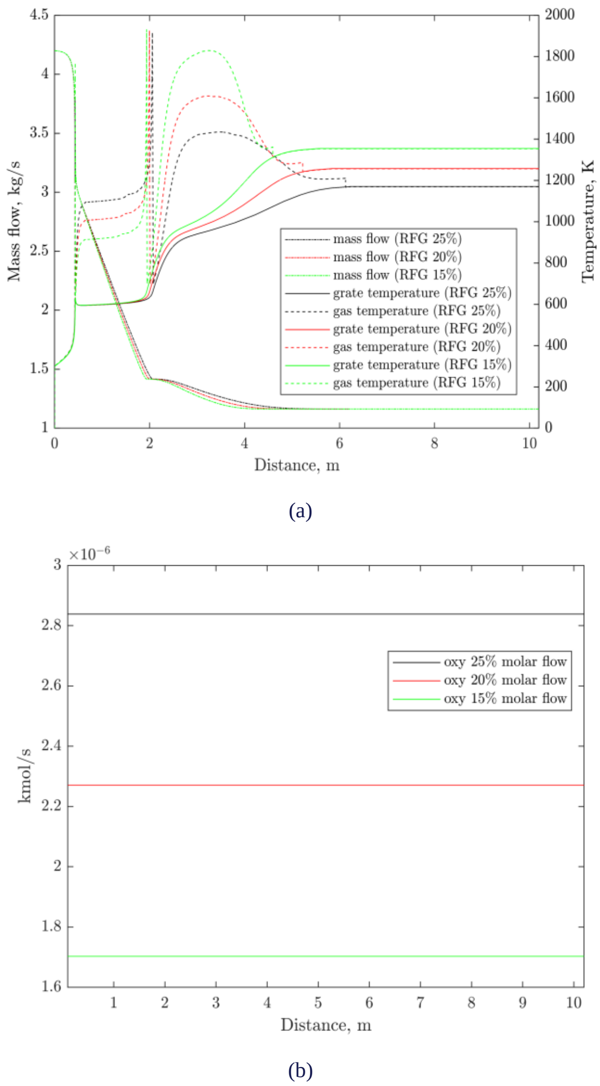


Fig. 10. a) Temperature of the grate and intermediate zone, and the mass flow of the fuel as a function of grate length;
b) Oxidant distribution along the grate.

the radiative heat transfer profile for the oxy-fired system in this case is more similar to air combustion than that predicted in the first studied case (compare to Fig. 7). Similarly, Figure 10 displays the temperature of the grate and intermediate zone, and the mass flow of waste as a function of grate length for considered ratios of flue gas recirculation. The results imply that the use of recirculated flue gas for evaporation and pyrolysis processes is feasible. Limiting oxygen slightly extends the process and significantly decreases the temperature in the combustion chamber.

Regarding the oxygen demand in the second case studied, the required amount of oxygen in the process decreased significantly, as shown in Table 6. This results in a lower consumption of electricity to power the air separation unit, which is employed to produce pure oxygen. As various studies have shown [7,51], the ASU is the most energy-intensive device in the oxy-fuel combustion systems. Therefore, in studies on oxy-waste incineration, the key parameter that will allow the selection of the optimal oxidant distribution strategy should be the oxygen demand.

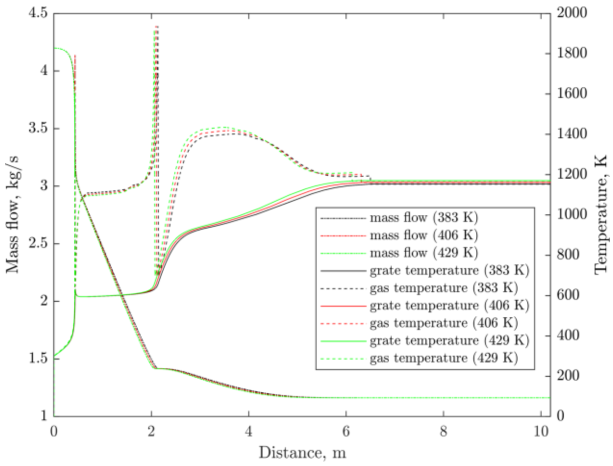


Fig. 11. Temperature of the grate and intermediate zone and the mass flow of the fuel as a function of grate length.

4.2.3. Effect of oxidizer temperature

In the last case, we analysed the influence of the oxidizer temperature on the process. We selected the conditions used in the second case (with the 25% of recirculated flue gas) and investigated three different temperatures of 383 K, 406 K and 429 K. The results presented in Fig. 11 indicate that the temperature of the oxidiser does not affect the process significantly.

5. Conclusions

This study presents the first attempt at mathematical modelling of real-scale oxy-waste incineration, which is a scientific novelty of this work. As a result, the 1D model of oxy-MSW combustion in a grate furnace is developed and analysed. The processes that were considered on the grate comprised waste drying, pyrolysis, the heterogeneous reactions of char and O_2/CO_2, based on the chemical kinetics, as well as homogeneous reactions between gases in the intermediate zone (above the grate). Besides, heat and mass transfer between the gas and solid phases are comprised.

The presented results showed that combustion parameters such as temperature and the duration of the process highly depend on oxidant composition:

- Increased content of oxygen in the supplied gas shortens the combustion process by around 30–50%.
- Increased content of oxygen elevates the temperature in the gaseous reactions area.
- Increased content of oxygen elevates the temperature in the grate.

Table 6. Oxygen demand for different oxy-fired conditions.

Parameter	Unit	Value		
RFG ratio	%	15	20	25
Total oxygen demand	kmol/s	0.0290	0.0232	0.0174
Share of oxygen in the oxidant	%	25		

- The study also confirmed that flue gas recirculation effectively control the temperature of the process.
- Moreover, the results indicate that the use of recirculated exhaust gases as an oxidant is sufficient for the drying and pyrolysis process.

Thus, oxy-fuel combustion of waste in a grate furnace can provide improved burnout and higher temperature with a sustainable ‘CO_2-less’ thermal conversion of fuel.

Results will be useful especially for the design purposes of the oxy-MSW combustion process since they show the duration of the various stages of waste incineration, the amount and composition of the obtained products, as well as the approximate temperature of the gaseous and solid phases depending on the used oxidant.

Acknowledgements

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