A novel approach for the numerical analysis of waste-to-energy plants

F Arpino¹, G Buonanno¹, G Cortellessa¹, M. Costa¹, M Dell’Isola¹, N. Massarotti² and F Zuena¹

¹ Department of Civil and Mechanical Engineering, University of Cassino and Southern Lazio, via G. Di Biasio 43, Cassino, Italy
Corresponding author e-mail: g.cortellessa@unicas.it
² Engineering Department, University of Naples “Parthenope”, Isola C4, Centro Direzionale di Napoli, 80143 Napoli, Italy
³ National Research Council of Italy (CNR), Istituto Motori, Viale Marconi 4, Napoli, Italy

Abstract. In this paper the authors present a simplified 0D-3D approach for modelling operating conditions of a waste-to-energy plant. This innovative methodology combines a 0D lumped parameters model, able to describe the processes of solid and gaseous combustion and the heat transfer within the first radiant channel, with a detailed 3D CFD simulation of the thermo-fluid-dynamic field within the plant combustion chamber. Besides, results from the 0D model allow the definition of input data and boundary conditions for detailed 3D CFD simulation of the thermo-fluid-dynamic field within the plant combustion chamber. In this way, the T2S temperature can be determined using a more efficient and complete methodology. The developed numerical tool, does not employ correlations based on empiric observations or on experimental data regressions and, being phenomenological, is generally applicable to any waste-to-energy plant, and is here applied for the characterization of different operating conditions of an Italian WTE. The analysis allows the verification of the constraints imposed by the European legislation on the temperature of the combustion products and the identification of any issues related to the plant operation. Input parameters are determined from measurements and the obtained numerical results are validated against experiments showing a good agreement.

1. Introduction

Energy recovery from incineration is an important part of the waste management process, although attention is to be devoted to the environmental impact of waste-to-energy plants. In order to avoid the formation of pollutants a proper combustion control is needed. In fact, in the last decades research activity showed that particulate carbon act as major carbon source for dioxins, that inorganic chlorides act as chlorine source, and that the presence of oxygen is essential [1]. Favoured precursors for dioxins formation are the products of incomplete combustion. Their reduction by a proper combustion control significantly reduces dioxin formation. To this aim, European legislation 2000/76/CE prescribes that, for non-hazardous wastes, the temperature of the gaseous combustion products, referred in the following as T2S, must be kept above 850 °C for at least 2 seconds [2, 3].

The respect of the imposed temperature constraint would allow thermal destruction of dioxin precursors. Nevertheless, it would require the ability to follow any fluid particle in the combustion chamber for at least 2 seconds, measuring its temperature at the same time. Since such measuring approach is unfeasible, the T2S is usually experimentally estimated performing temperature measurements in correspondence of given combustion chamber location, basically assuming that fluid particles follow a straight path with no recirculation. In a WTE plant operation, the T2S is usually continuously verified in situ by employing simplified 0D models, typically based on the use of empiric correlations obtained from measurements performed on similar plants, and assuming a reference biomass fixed composition. Such an approach offers the advantage to be relatively simple and not demanding from the computational point of view. Nevertheless, its ability to actually predict the T2S temperature depends on the fluid velocity field within the combustion chamber and
obviously on the actual Refuse Derived Fuel (RDF) composition [4]. The uncertainty affecting the predicted temperature may be significantly large, forcing the plant to operate at higher temperature in order to respect legislation prescription. The necessity to calculate the \( T_{2S} \) temperature using a more efficient and complete methodology prompted the authors to develop a general numerical model able to predict steady operating conditions of the WTE plants.

In the present paper the authors propose a novel thermodynamic approach for the analysis of WTE plants. This innovative methodology combines a simplified thermodynamic 0D lumped parameters model, able to describe the processes of solid and gaseous combustion and the heat transfer within the first radiant channel, with a detailed 3D CFD simulation of the thermo-fluid-dynamic field within the plant combustion chamber. The general 0D model is not based on the use of empirical or semi-empirical correlations, deriving from experimental data regressions and calibrated for a specific co-incineration plant, but on the actual Refuse Derived Fuel (RDF) composition and the real flow rates and reagents temperature (primary and secondary air) in input to the system. Besides, results from the 0D model allow the definition of input data and boundary conditions for detailed 3D CFD simulation of the thermo-fluid-dynamic field within the plant combustion chamber. In this way the \( T_{2S} \) temperature can be determined using a more efficient and complete methodology. The developed numerical tool is here applied for the characterization of different operating conditions of an Italian WTE. The plant produces an electric power of about 11 MW and a thermal power of about 47 MW. The combustion chamber is a grate fired boiler, with three vertical channels and energy recovery, able to produce about 60 t/h of water vapour at a pressure of about 60 bar.

The analysis allows the verification of the constraints imposed by the European legislation on the temperature of the combustion products and the identification of any issues related to the plant operation. An experimental campaign was conducted during which data from existing instrumentation installed on the combustion chamber of the plant was collected. Besides, during the campaign the chemical characteristics of the RDF actually used to feed the plant were analysed and proper uncertainty analysis was conducted on the collected experimental data.

The input parameters were determined from measurements and the obtained numerical results were validated against experimental data in terms of data compatibility, showing a good agreement. The estimation of the measurement uncertainty associated to the results of the proposed model was performed by calculating suitable sensitivity coefficients and by applying the well-known uncertainty propagation law. Referring to an operating period of one week: i) all operating parameters from the plant instrumentation were collected; ii) a detailed composition analysis of the RDF was conducted; iii) additional temperature measurements were performed in the first channel of the combustion chamber; iv) a general simplified thermodynamic model for waste-to-energy plants was formulated; v) a detailed CFD analysis was performed. Obtained results were validated against collected experimental data.

2. The proposed 0D-3D modelling approach

The simplified 0D-1D model is applied to the first channel of the combustion chamber, subdivided in the following 4 control volumes (Figure 1): i) RDF gasification control volume; ii) heat exchange volume placed upstream the gaseous combustion; iii) combustion of gaseous products; iv) heat exchange volume placed downstream the gaseous combustion region. The RDF gasification process is modelled assuming thermodynamic equilibrium, according to the following global reaction:

\[
CH_xO_yN_z + wH_2O + m(O_2 + 3.76N_2) = n_{H_2}H_2 + n_{CO}CO + n_{CO_2}CO_2 + n_{CH_4}CH4 + \left(\frac{z}{2} + 3.76m\right)N_2 \tag{1}
\]

where \( CH_xO_yN_z \) represents the equivalent chemical formula of the feedstock where \( x, y \) and \( z \) represent the number of atoms of hydrogen, oxygen and nitrogen while \( w \) and \( m \) represent the mole number of water and oxygen for each mole of carbon. Mass balance for carbon, hydrogen and oxygen are solved. Besides, thermodynamic equilibrium equation is solved for the Boudouard reaction, water-shift and methane oxidation [5]. Finally, the gasification temperature is calculated by solving the energy conservation equation, taking into account heat from reactions and radiation to the surrounding combustion chamber. The heat transferred between gaseous products and the working fluid (water vapour) is calculated using the heat exchangers equation, numerically estimating the global heat transfer coefficient, \( U \) (Wm\(^{-2}\)K\(^{-1}\)), on the basis of the characteristics of the solid walls of the combustion chamber (control volume VC1). Finally, the combustion of gaseous products (control volume VC2) is considered, allowing the calculation of exhaust composition and of the heat power released. The energy contribution resulting from the gaseous combustion can be calculated by
the knowledge of the syngas composition (deriving from the resolution of the control volume VC0). For this purpose, the following total reactions of oxidations were considered:

\[
\begin{align*}
H_2 + \frac{1}{2} O_2 & \rightarrow H_2O \quad \text{\( \Delta H_{\text{H}_2}^{\text{Comb}} = -241700 \text{ J mol}^{-1} \)} \\
CO + \frac{1}{2} O_2 & \rightarrow CO_2 \quad \text{\( \Delta H_{\text{CO}}^{\text{Comb}} = -283000 \text{ J mol}^{-1} \)} \\
CH_4 + 2O_2 & \rightarrow CO_2 + 2H_2O \quad \text{\( \Delta H_{\text{H}_2}^{\text{Comb}} = -802702 \text{ J mol}^{-1} \)}
\end{align*}
\]

In addition to the combustion reactions, the shift water reaction was used:

\[
\text{CCO + } H_2O \leftrightarrow \text{CO}_2 + H_2 \quad \text{\( \Delta H_{\text{w}}^{\circ} = -41200 \text{ J mol}^{-1} \)}
\]

The chemical kinetics was modelled by using the following relations [18, 19]:

\[
\begin{align*}
H_2 + \frac{1}{2} O_2 & \rightarrow H_2O \quad r_1 = k_1[H_2][O_2] \quad k_1 = 5.26 \times 10^{19} e^{20500/T} \\
CO + \frac{1}{2} O_2 & \rightarrow CO_2 \quad r_2 = k_2[CO][H_2O]^0.5[O_2]^0.25 \quad k_2 = 3.16 \times 10^{12} e^{21664/T} \\
CH_4 + 2O_2 & \rightarrow CO_2 + 2H_2O \quad r_3 = k_3[CH_4][O_2] \quad k_3 = 2.552 \times 10^{17} e^{11196/T} \\
CO + H_2O & \leftrightarrow CO_2 + H_2 \quad r_{\text{ws}} = k_{\text{ws}} \left( [CO][H_2O] - \frac{[CO_2][H_2]}{k_{\text{ws,eq}}} \right) \quad k_{\text{ws}} = 2.778 \times 10^{3} e^{1511/T} \quad k_{\text{ws,eq}} = 0.022 e^{4179/T} 
\end{align*}
\]

The reaction rate, expressed in moles per unit of time and volume, are indicated with \( r_1, r_2, r_3 \) and \( r_{\text{ws}} \). The equations (3) and (4) are solved using a time-variant explicit procedure. The reactions resolution in gaseous phase allows the calculation of both the thermal power applied by the combustion reactions and the composition of the exhausts (control volume VC3) by the same relations used in the resolution of the control volume VC1.

The 3D detailed CFD model described the pressure, velocity and temperature fields in the combustion chamber of the waste to energy plant by solving the well-known mass, momentum and energy conservation equations for compressible fluids. Turbulence is modelled using the Reynolds Averaged Navier Stokes (RANS) approach and the realizable \( k-\epsilon \) turbulence model. Boundary conditions for 3D simulations are obtained from simplified model results. In particular, gasification temperature and syngas mass flow rate are assumed in correspondence of the primary air inlet; the global heat transfer coefficient, \( U \) (W m\(^{-2}\) K\(^{-1}\)), alongside with geometrical and thermophysical characteristic of solid walls of the combustion chamber (thickness and thermal conductivity of refractory bricks) are assumed in correspondence of non-adiabatic walls; temperature and mass flow rate mixture of secondary air and recirculating exhausts (if present) are assumed at the secondary air inlet sections. Besides, gaseous combustion process is modelled by imposing in the secondary air injection zone a proper heat source terms, obtained from the simplified 0D-1D model. Finally, radiation is modelled by evaluating exhaust emissivity on the basis of composition obtained from simplified calculations. A schematic of the employed control volumes and the main interaction and between 0D-1D and 3D models are reported in Figure 1.
3. Results

The proposed 0D-3D numerical model was applied for the characterization of different operating conditions of an Italian WTE. As previously introduced, a 5-days experimental campaign, was conducted aimed at collecting information about operating temperatures, reactants and products flow rates, and RDF composition. An additional silicon carbide bar equipped with four thermocouples was also introduced within the combustion chamber at a distance of about 6 m from the secondary air injection zone. In the following, the validation and the obtained results deriving from the application of the thermodynamic 0D model and the 3D numerical model are illustrated.

3.1 Thermodynamic 0D model

The 0D model, in addition to providing the boundary conditions necessary for the resolution of the most complex 3D simulations, can be employed for the determination of T_{2S} correlations, directly implemented to the DCS (Distributed Control System) of the waste-to-energy plant. The results obtained by the application of the 0D model to the selected Italian plant, have been compared with measurements available from instruments installed on the combustion chamber. The collected experimental data allowed the complete definition of the input parameters for the thermodynamic model, with related measurement uncertainty. Obtained results were validated in terms of averaged temperature in correspondence of the instrumented bar and on the top of the combustion chamber, and of the oxygen and water vapour content in the exhausts. In particular, a detailed parametric analysis was conducted and the results were compared with experiments in terms of data compatibility, taking into account measurements uncertainty. Figure 2, as an example, shows the dependence of some model results from the carbon mass fraction in the dry RDF. In particular, Figure 2(a) reports the syngas composition, while Figure 2(b) describes the variation of the temperature T_{2S}, the average temperature in correspondence of the instrumented bar, T_B, the mean temperature at the chamber top, T_C, the gasification temperature, T_{RDF}, and the distance, H_{2S}, travelled by the exhaust in the time of 2 seconds. The thermodynamic model validation is shown in Figure 3. In particular, the obtained results are compared with experimental data in terms of mean temperature at the top of the combustion chamber (left) and oxygen content at the exhaust (right). The error bars, in the figure, represent the estimated uncertainty. Numerical and experimental data are compatible for all the considered plant operating conditions.
Figure 2. Schematic representation of the proposed general thermodynamic model.

Figure 3. Thermodynamic OD model validation.

Comparisons between measurements and numerical results from thermodynamic OD model in terms of normalized temperature as a function of normalized load (produced water vapour) are available in Figure 4 at different height of the combustion chamber, normalized with respect to the distance between the last secondary air injection section and the ceiling of the chamber. Discrepancy between measurements and numerical results is equal to 2.2% in average, a median of 2.6% and a peak of 6.0%.

Figure 4. Comparison between experiments and results from 0D-1D model.
3.2 3D numerical model

3D numerical simulations were performed reproducing the operative conditions of the plant in the reference period. Figure 5a shows an example of computational domain obtained from 3D simulation. In particular, starting from the first three radiant channels, the plane of geometric symmetry and the boundary conditions were identified and shown in the figure. The calculation domain was essentially limited to the first radiant channel of the plant, in addition to part of the second radiant channel, necessary to reproduce, in an accurate way, the area of passage of the exhausts from the first to the second channel.

![Image of computational domain](image1.png)

**Figure 5.** Example of the computational domain used for the numerical simulations (a); global heat transfer coefficient $U$ at the walls of the combustion chamber (b).

The boundary conditions used in the 3D numerical simulations were obtained from the application of the 0D model to the plant operating conditions during the selected 5-days reference period. The data obtained from the 0D model and used as input for the 3D simulations are shown in Table 1. In Figure 5b the global heat transfer coefficient $U$ at the walls of the combustion chamber is also reported. Because the chemical analysis of the RDF composition was only performed in one of the 5-days reference period, for brevity, only CFD results related to this day are reported. The numerical simulations were performed by using a computational grid composed by 289271 nodes and 1574817 tetrahedral elements. In order to ensure results independence from employed grid, a mesh sensitivity analysis has been conducted choosing a grid with an error of less than 5% at the ceiling of the first radiant channel. In Figure 6, two representations of the adopted grid are reported in which three sections on the $xz$ plane and one section on the $xy$ plane are highlighted. In particular, in Figure 5(a) the grid is reported for a section at a distance of 0.5 m from the wall, while in Figure 5(b) the grid is reported for a section at a distance of 2.5 m from the wall.

3D numerical simulations were performed reproducing the operative conditions of the plant in the reference period. In Figure 7 the streamlines, the velocity contour and the temperature contour are reported for the selected day. In all the investigated operating conditions a recirculation zone, in correspondence of the front wall of the computational domain (wall containing the nozzles suppling the upper secondary air), was found. The extension of this zone is not only due to the syngas and secondary air flow rate in input to the domain, but also to the local temperature distribution, from which the fluid density depends (Figure 7a).
Figure 6. Computational grid adopted for the 3D numerical simulations, composed by 289271 nodes and 1574817 tetrahedral elements.

Table 1. Input and Boundary conditions used for the 3D simulation and obtained by the 0D model resolution.

| Boundary conditions                                      | Value   |
|----------------------------------------------------------|---------|
| Syngas volumetric flowrate in input ($Nm^3 \cdot h^{-1}$) | 58090   |
| Average gasification temperature ($K$)                    | 1341    |
| Equivalent syngas temperature in input ($K$)              | 1265    |
| Thermal power given by the gaseous combustion ($MW$)     | 27.145  |
| Secondary air volumetric flow rate (front upper) ($Nm^3 \cdot h^{-1}$) | 15455   |
| Secondary air volumetric flow rate (front lower) ($Nm^3 \cdot h^{-1}$) | 3312    |
| Secondary air volumetric flow rate (rear) ($Nm^3 \cdot h^{-1}$) | 15576   |
| Secondary air input temperature ($K$)                     | 298     |

In Figure 7b, the velocity contour evaluated in different sections on the xy and xz planes is illustrated. From the analysis of this figure, it is possible to observe that, due to the presence of the recirculation zones previously highlighted, the flow presents a higher velocity in the middle of the channel, while it becomes significantly slower approaching towards the front wall of the domain. This velocity variation is due to the injection of secondary air (velocity in input is of the order of $10^2$ m/s). The velocity field within the domain depends from the input conditions but also from the temperature distribution. The behavior of the velocity field, highlighted above, allows the hot gas flow mainly laps the rear wall of the first radiant channel. The effects of this characteristic are clearly evident in Figure 7c, where it is possible observe that the rear wall reaches a maximum temperature over 100°C higher than that of the front wall.

In Figure 7c, the temperature contour is illustrated. From this figure, it is possible to observe the effect of the thermal power generated by the gaseous combustion, modelled through a generation term uniformly distributed in the volume. Since the inlet velocity of the upper front secondary air is significantly higher than the inlet velocity of the other secondary air injectors, it is reasonable to expect that the chemical conditions favorable to the gas combustion will occur closer to the rear wall of the domain. The hot fluid flow impacts the rear part of the first radiant channel causing a significant increase in temperature with respect to the other walls covered with refractory material. Finally, in Figure 8 comparison between numerical and experimental data in correspondence of the ceiling of the first radiant channel are illustrated.
Figure 7. Streamlines (a), velocity contour (b) and temperature contour (c) obtained from the numerical simulation.

Figure 8. Comparison between numerical and experimental data evaluated in correspondence of the ceiling of the first radiant channel

4. Conclusions

The authors propose a general 0D-3D model for the description of waste-to-energy plants fed by RDF. An innovative methodology is proposed, combining a thermodynamic 0D parameters model, able to describe the processes of solid and gaseous combustion and the heat transfer within the first radiant channel, with a detailed 3D CFD simulation of the thermo-fluid-dynamic field within the plant combustion chamber. The simplified model proves being a good compromise solution between results reliability, flexibility and computational saving. As a further development, the thermodynamic model also allows the definition of the input parameters for a detailed non reacting 3D CFD simulation of the first vertical channel of the combustion chamber. Besides simulations, a detailed experimental campaign is conducted, which allows the model validation. The proposed simplified model is not based on empirical or semi-empirical correlations, but it is of phenomenological type, since it is based on balance equations for the thermodynamic variables and the chemical equilibrium hypothesis between participating species. Numerical results have been compared with experiments showing a very good agreement. Three dimensional CFD simulations allow the prediction of $T_{2S}$ temperature taking into account actual 3D characteristic of the flow. The comparison of results with detailed CFD simulations showed that the model presents a good reliability and flexibility, with a very low computational cost.
5. References

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