

Article

Numerical Simulation of the Combustion of a Coal Char Particle Spherically Shrinking in a Drop Tube Furnace

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Featured Application: The simple model which is proposed could be considered to simulate in an efficient way combustion processes performed in a drop tube furnace, as it also gives access to variations of local quantities, remaining much simpler than other models.

Abstract: Modeling the combustion of a coal char particle in a drop tube furnace is still a challenge, although different models are available in the literature. A simple model is proposed here which considers the combustion of a single coal char particle in a drop tube furnace, assuming that the shrinking particle remains spherical during its combustion, among other hypotheses. This model is much simpler than most available ones, as it is based on two differential equations respectively describing the evolution with respect to the time of the particle temperature and that with respect to the particle radius of the oxygen concentration inside the particle. This model further gives access to local quantities which allow characterizing the combustion process. The simulations performed with this model are validated mainly through comparisons between the experimental and simulated particle temperatures under three constant regulation temperatures of the drop tube furnace.

Keywords: spherical coal char particle; shrinkage; drop tube furnace; combustion; modeling



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1. Introduction

Modeling the combustion process of coal particles and of coal char particles in furnaces or boilers is still a complicated task, although such a combustion process was already analyzed and simulated by many authors for a long time and through different models or tools. The combustion of coal particles may be decomposed in two main stages, which can superimpose: a devolatilization one, leading to coal char particles, and a combustion one. A complete review of the different models for coal pyrolysis, combustion and gasification was presented in [1], together with the corresponding mechanisms and structure modifications. A Thiele analysis and a random pore model were combined to describe the combustion of coke particles in an atmospheric fluidized bed combustor [2]. A model was proposed by Mitchell to simulate the physical changes occurring during the combustion of char particles [3]. Local values of the parameters were considered here, which allow the local use of the random pore model for the description of the evolution of the specific surface area. The devolatilization of a single coal particle and the combustion of the residual char were modeled in [4]. For the devolatilization stage, the authors assumed that the activation energy obeys a Gaussian distribution and they wrote an energy balance which describes the evolution of the temperature inside the spherical particle (with fixed radius), with respect to time. For the further char combustion stage, the authors used the pore evolution model introduced in [5]. They wrote conservation laws for the gas species, a total molar balance of gas mixture, an energy balance and a total mass balance of carbon in the spherical char particle. In the gas boundary layer, they wrote conservation equations. For the resolution of this large system of evolution equations, the authors built an integrated Fortran code.

The combustion of a gasified semi-char in a drop tube furnace was analyzed in [6], through a pore development process and the use of the Thiele modulus method, based on the following expression of the effectiveness factor:

$$\eta = \left(\coth(3\Phi) - \frac{1}{3\Phi} \right) \frac{1}{\Phi}, \quad (1)$$

where Φ is the Thiele modulus, and on a simple expression of the oxygen concentration at the particle surface. Here, the authors assumed a constant particle temperature. A random pore model with intraparticle diffusion was introduced in [7], to describe the combustion of char particles. A coal combustion model was presented in [8], which was based on a kinetic model, the chemical reaction rate being taken as a function of the coal intrinsic reactivity and fuel mass for a global reaction of order n . Different models of coal combustion were compared in [9]. A reduced and one-dimensional model was proposed in [10], to simulate the combustion of a spherical char particle. This model was based on a constant particle radius and uniform values of the different structural parameters within the particle and at any time of the combustion process, allowing the use of the Thiele modulus method, through Equation (1). The authors evaluated the impact of ash on the combustion behavior. More recently, the characteristics of char burnout of a biomass/coal blend were analyzed through a simplified single particle reaction model [11]. The authors here defined an intrinsic reactivity coefficient as a function of the char conversion rate and of the effectiveness factor which involves the Thiele modulus, according to Equation (1). In [12], the authors analyzed and simulated the combustion of a coal char particle in a drop tube furnace under different mixtures of O_2 , CO_2 , Ar and N_2 . Their model was based on a heat transfer equation and two heterogeneous reactions. They computed the carbon consumption rate. For the effectiveness factor, the authors used Equation (1). The spherical particle was allowed to shrink keeping its spherical symmetry. For the validation of their model, the authors compared their simulations with experimental carbon conversion values. In [13], the authors considered the combustion of a single coal char particle in a drop tube furnace under O_2/H_2O conditions. They considered two reactions for the char- O_2 combustion reaction, two for the char- H_2O combustion reaction, three for the char- H_2O gasification reaction and six further gasification or combustion reactions. They associated kinetic relationships to these reactions. They then wrote a total molar balance of gas mixture, a heat transfer equation and a mass transfer equation. They used the Maxwell–Stefan diffusion equation for the mass transfer in a multicomponent system (O_2 , CO, CO_2 , H_2O and H_2). They added initial and boundary conditions. For the resolution of their model, the authors used the finite volume method. For the validation of their model, they compared their simulations with experimental data concerning the global carbon conversion.

More complex models are proposed in the literature to simulate the combustion of char particles falling in a drop tube furnace, which use Computational Fluid Dynamics (CFD) tools. The purpose here is to also simulate the trajectory of the particle during its fall in the drop tube furnace. Such models require an appropriate meshing of the reactor and dedicated software to solve the complex model, which usually involves different chemical reactions [1]. Numerical simulations of coal combustion performed in three furnaces were described in [14]. Mainly focusing on the devolatilization stage, the authors used the tabulated–devolatilization–process model developed in [9] and the FLASHCHAIN model developed for example in [15], to simulate this devolatilization stage. In [16], the authors simulated the combustion of spherical and non-deformable coal particles in a large-scale laboratory furnace. They distinguished between the devolatilization and char combustion stages. In [17], the Large Eddy Simulation tool was used to simulate the combustion of pulverized coal in a large-scale laboratory furnace. The authors also distinguished between the devolatilization and char combustion stages. They used an in-house code to solve the systems of equations. In [18], a flamelet model was proposed for coal combustion involving a quite similar tool. The oxy-fuel combustion of Victorian brown coal in a drop

tube furnace and in a 3 MW pilot scale burner was simulated in [19] with CFD tools. The authors here presented a complete set of equations and they considered a particle random trajectory model.

In the present study, a simple model is proposed to simulate the shrinking behavior of a spherical coal char particle burning during its fall in a drop tube furnace. The model thus focuses on the “second” stage of the combustion of a coal particle under high temperature ramps. It is based on two main hypotheses: the non-uniformity of structural quantities (particle density, porosity, mean pore radius and specific surface area) and the preservation of the spherical symmetry of the coal char particle during its combustion. The model mainly consists of two differential equations which respectively describe the evolution with respect to time of the particle temperature and that with respect to the particle radius of the oxygen concentration inside the particle. This model is solved using an in-house Fortran code, thus requiring no commercial or CFD software, or CFD skills. It remains much simpler than many available models especially that based on CFD tools. Instead of Fortran, every scientific software able to solve partial differential equations can be used. To validate the model, comparisons between the experimental and simulated temperatures of a coal char particle introduced in the drop tube furnace are first proposed at three constant regulation temperatures of the reactor (1100, 1200 and 1300 °C). Comparisons of the simulated global carbon conversion with few experimental data given in the literature are also presented. The Thiele modulus, which governs the oxygen transfer within the particle, is computed in terms of the oxygen flux at the particle surface. In the present study, the oxygen concentration is computed within the whole particle. The Thiele modules gives access to the effectiveness factor of the particle which is used to obtain the oxygen flux entering the particle. The model which is proposed gives access to local quantities which allow characterizing the combustion behavior of the coal char particle. Despite its simplicity, this model is more complete than that presented in many studies. This model improves the preceding one presented in [20], as the particle is allowed to shrink in the present study, but keeping its spherical symmetry.

2. Materials and Methods

2.1. Characterizations of the Coal and Resulting Coal Char

A South African bituminous coal was used to produce coal char particles through pyrolysis experiments performed in an adapted configuration of a drop tube furnace. The coal particles were crushed and sieved to a 36–72 µm size fraction, with a mean diameter of 50 µm. Ballester et al. pointed out the importance of accounting for the size distribution of coal particles when modeling their combustion in an entrained flow reactor [21]. Accounting for the size distribution of the coal particles was also pointed out in [22].

The coal char particles were then burnt in a slightly modified configuration of the drop tube furnace.

The proximate and ultimate analyses of the coal and of the resulting coal char are gathered in Table 1.

The higher heating value of the coal used in the present study was determined equal to 27.3 MJ.kg^{−1}. The density of the coal char material was evaluated equal to 296.6 kg.m^{−3}. The specific surface area of the coal char was measured equal to 131,800 ± 1300 m².kg^{−1} according to the precision equal to 1%, as indicated in the operating manual.

The proximate analyses show that during the pyrolysis experiments applied to the coal particles, their volatile matter and moisture contents are almost totally removed. Consequently, the ash and fixed carbon percentages increase in the resulting coal char particles. The hydrogen and oxygen percentages are slightly lower and the carbon percentage is higher in the coal char particles than in the coal ones.

Table 1. Proximate and ultimate analyses of the South African coal considered in the present study and of the coal char produced from the coal particles through pyrolysis experiments in the drop tube furnace.

	Coal	Coal Char
Proximate analysis (wt%, ar ¹)		
Volatile matter	24.0	0.7
Ash	13.8	20.0
Fixed Carbon	54.7	78.5
Moisture	7.5	0.8
Ultimate analysis (% , daf ²)		
C	67.64	76.63
H	3.77	0.89
O ³	26.02	20.69
N	1.81	1.26
S	0.76	0.53

¹ As received. ² Dry and ash-free basis. ³ Computed by difference.

2.2. Experimental Conditions for the Pyrolysis and Combustion Experiments

The configurations of the drop tube furnace used for the pyrolysis of the coal particles and for the combustion of the resulting coal char particles are presented in Figure 1.

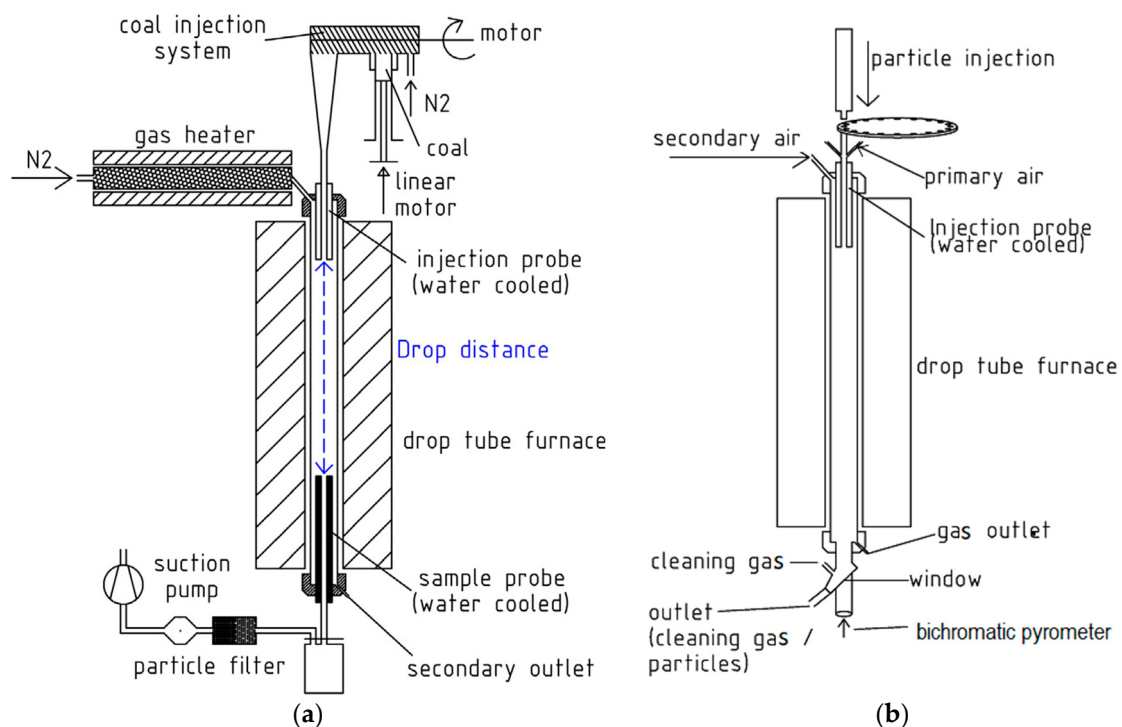


Figure 1. A schematic representation of the drop tube furnace used for the pyrolysis experiments applied to coal particles (a), and for the combustion of the resulting coal char particles (b).

The silica–alumina reactor of the drop tube furnace is 1.7 m high and its radius R_r is equal to 3.5 cm. This reactor is placed inside a furnace whose temperature is controlled. For the combustion experiments on the coal char particles, three constant regulation temperatures of the reaction zone of the drop tube furnace were considered: 1100, 1200 and 1300 °C.

The first main difference between the two configurations of the drop tube furnace deals with the injection system. For the pyrolysis experiments, the coal particles were injected through an injection probe at a rate equal to $17 \times 10^{-13} \text{ kg.h}^{-1}$, Figure 1a, together

with a nitrogen flow of 400 L.h^{-1} pre-heated at 1300°C . The drop distance was 1 m length. Concerning the combustion experiments, for each injection sequence, 2 mg of coal char particles were injected through a water cooled injector with a primary gas flow (40 L.h^{-1}), under an oxidative atmosphere (12% oxygen, balance nitrogen). Then, the coal char particles were entrained by a secondary nitrogen flow (360 L.h^{-1}) preheated at 900°C , Figure 1b.

Concerning the outlet in the case of the pyrolysis experiments, the coal char particles were collected through a sample probe which was water cooled, Figure 1a. For the combustion experiments, the particle temperature was recorded by a two-color pyrometer IMPAC ISR 12-LO, placed at the bottom of the drop tube furnace and vertically pointing to the reaction zone of the drop tube furnace, Figure 1b. This particle temperature measured during its fall in the reactor is the only experimental data which are available. For a regulation temperature equal to 1200°C , a shift of 75°C was observed between the lowest and the highest maxima of the particle temperature, with a mean temperature equal to 1353°C . This roughly corresponds to an uncertainty equal to 38°C , which is in agreement with Solomon et al. who wrote in [23] that temperature measurements by optical methods are given within an uncertainty equal to $\pm 50^\circ\text{C}$, when the particle is observed along its overall trajectory.

For the combustion experiments of the coal char particles, at least nine injections were performed.

2.3. Hypotheses of the Model Accounting for the Coal Char Combustion Experiments

The hypotheses of the model proposed in the present study are the following:

Hypothesis 1: A mean velocity u_g of the injected gas is considered in each horizontal section of the reactor, which is calculated in terms of the gas flow F_g^0 and gas temperature T_g , according to the formula: $u_g = (T_g/298)F_g^0 / (\pi(R_r)^2) \text{ (m.s}^{-1}\text{)}$. The gas temperature T_g is measured along the reactor axis and set in the model as a function of the particle position.

Hypothesis 2: The coal char particles may obey a transient velocity regime during a very short time length after their injection, but it is assumed that they are carried through the reacting zone of the drop tube furnace at the gas velocity.

Hypothesis 3: The coal char particles enter the reactor at 323 K .

Hypothesis 4: The coal char particles are supposed to keep their spherical symmetry during their fall in the drop tube furnace.

Hypothesis 5: A mean value of the initial coal char particle radius is considered: $R_p(0) = 65 \times 10^{-6} \text{ m}$, as determined through measurements.

Hypothesis 6: Due to the small radius of the particle, the particle temperature $T_p(t)$ is supposed to be uniform within the particle at any time t of the combustion process, in agreement with the discussion in [23].

Hypothesis 7: The heat transfer modeling includes convection between the particle and gas, radiations between the particle and reactor walls and heat release by particle combustion.

Hypothesis 8: The ash presence inside the coal char particle is accounted for, which is supposed to be homogeneously distributed within the particle at any time of the combustion process.

Hypothesis 9: The oxygen diffusion coupled with the reaction within the porous structure is modeled to determine the local oxygen concentration along the particle radius at any time of the combustion process. External diffusional limitations through a boundary layer are also accounted for. Due to oxygen internal diffusion limitations, the combustion is not homogeneous within the particle along the combustion process. For the numerical resolution of the system of equations, the initial particle is divided into $N = 500$ concentric volume elements, with equal thickness: $dr = R_p(0)/N = 1.3 \times 10^{-7}$ m. The volume element which lies between the spheres of radii $(i - 1)dr$ and idr is labeled with its subscript i , $1 \leq i \leq N$. For the oxygen diffusion model, a unique pore model is locally used within every volume element of the spherical particle, which allows estimating the different local pore radii and their evolution versus time. The different physical quantities (particle density, carbonaceous material density, porosity, pore radius and specific surface area) are supposed to be initially uniformly distributed within the particle.

Hypothesis 10: The quasi-stationarity of the oxygen diffusion process is assumed, due to the very small values of the time derivatives (corresponding to accumulations terms) within the diffusion differential equation.

Hypothesis 11: The diminution of the particle radius along the combustion process is accounted for, assuming that the outer volume element of the particle labelled $N_s(t)$, with $1 \leq N_s(t) \leq N$, is removed from the particle when the local carbon conversion in this volume element becomes higher than a chosen threshold: $(X_C)_{N_s}^{lim} = 0.99$. At the beginning of the combustion process, $N_s(0) = N = 500$. The radius $R_p(t)$ of the particle thus evolves with respect to the time parameter t according to the expression: $R_p(t) = R_p(0)N_s(t)/N$. Each time the outer volume element is removed from the particle, the number N_s of the remaining volume elements is reduced by 1, and the ash amount contained within this outer volume element is deduced from the current amount of ash within the particle.

Hypothesis 12: The evolution of the local surface specific area in every volume element of the particle is calculated following the random pore model proposed by Bhatia and Perlmutter, whose parameters are derived from experiments, [5]. This local specific area is supposed to grow up from $131,800 \pm 1300 \text{ m}^2.\text{kg}^{-1}$, for the initial coal char material, to the maximal value of $300,000 \text{ m}^2.\text{kg}^{-1}$.

Hypothesis 13: For the kinetic study of the carbon combustion, an order-reduced model is used, considering the single equation:



The three first hypotheses are more observations of the experimental setup.

The fourth hypothesis allows for using the spherical coordinates in the balance equation describing the evolution of the oxygen concentration within the particle, leading to a reduction of the number of spatial variables, whence to an easier resolution of this equation. In [24], the evolution of the shape of a coal particle during its combustion in a drop tube furnace was analyzed through high-speed imaging and image processing techniques. Two sizes of the coal particles were considered: 150–212 μm and 106–150 μm . The authors determined the aspect ratio of a particle as the ratio between the major axis to the minor one. For the smallest particle, this aspect ratio was measured between 1.1 and 1.8, with periodic variations that the authors attributed to rotations of the particle during its combustion. They also observed a diminution of the particle area during the combustion, which proves that the particle shrinks during its combustion.

Concerning the fifth hypothesis, a sensitivity analysis is performed in the present study with respect to few parameters and especially the particle radius. The impact of a variation of $\pm 20\%$ from the chosen value on the global carbon conversion is analyzed; see Section 3.

The sixth hypothesis concerning the uniformity of the particle temperature allows for describing the evolution of this particle temperature through an ordinary differential equation, whose resolution is much simpler than that of partial differential equations.

Hypotheses 4 and 6 allow the resolution of the proposed model without the use of any commercial or CFD code.

Hypothesis 7 simply expresses that the different modes of heat transfer are taken into account in the present model.

Hypothesis 8 is somehow usual in the present context.

Hypotheses 9 and 11 are classical ones when discretizing a spatial domain necessary for the resolution of differential equations, within the context of a spherical particle.

Hypothesis 10 is also a simplifying hypothesis, which allows a partial decoupling of the resolutions of the two differential equations of the model.

As indicated above, Hypothesis 12 refers to the known random pore model.

Different models were proposed for the kinetic study of the carbon combustion, together with the associated reaction rates and values of the kinetic parameters [3]. In [25], the authors proposed 18 reaction mechanisms for the combustion of carbonaceous materials under atmospheres including H_2O , CO_2 and O_2 , together with the corresponding reaction rates. Other reaction models than that proposed in Hypothesis 13 were tested during the present study, which involve more reaction mechanisms and parameters. However, no significant improvements of the simulations were observed when considering such more complicated reaction models.

A discussion concerning the effect of modeling assumptions used when simulating the combustion of pulverized coal through commercial codes was presented in [26]. The authors computed uncertainties associated to the variations of few parameters on the calculated particle mass and temperature.

2.4. Description of the Model Accounting for the Coal Char Combustion Experiments

Throughout the presentation of the model, no distinction will be introduced between the letters representing local and global quantities (see also the Nomenclature at the end of the manuscript). The variables attached to the quantities in the successive equations of the model certainly allow for understanding the local or global character of these quantities.

To start with the description of the model under consideration in the present study, the position of the particle is calculated as a function of the time parameter through the integral: $x_p(t) = \int_0^t u_g(s)ds$ (m), where u_g is the mean velocity of the injected gas, see Section 2.3, Hypothesis 1.

The evolution of the uniform particle temperature T_p with respect to time is governed by the differential equation:

$$\begin{aligned} & (m_C(0)(1 - X_C(t))C_{p,C} + m_{ash}(t)C_{p,ash})\frac{dT_p}{dt}(t) \\ & = 4\pi R_p^2(t)\varepsilon_p\sigma(T_{wall}^4(t) - T_p^4(t)) + 4\pi R_p^2(t)h(T_g(t) - T_p(t)) \\ & + (\tau(t)|\Delta_R H_{CO}^0|(t) + |\Delta_R H_{CO_2}^0|(t))\frac{\Phi_{O_2}(t)}{1+\tau(t)/2}, \end{aligned} \quad (3)$$

where $m_C(0)$ is the initial mass of carbon in the coal char particle, X_C the global carbon conversion, $C_{p,C}$ the calorific value of carbon, m_{ash} the ash mass within the particle, $C_{p,ash}$ the calorific value of ash, ε_p the char particle emissivity, σ Stefan–Boltzmann constant, T_{wall} the temperature of the reactor walls, h the convective heat transfer coefficient, $\Delta_R H_{CO}^0$ and $\Delta_R H_{CO_2}^0$ the enthalpies respectively expressed in terms of the particle temperature as: $\Delta_R H_{CO}^0 = -110.5 \times 10^3 - 6.38 \times (T_p - 298)$, $\Delta_R H_{CO_2}^0 = -393.5 \times 10^3 - 13.1 \times (T_p - 298)$ (J.mol⁻¹), Φ_{O_2} the oxygen molar flux at the particle surface and τ the ratio between the

instantaneous rates of CO and CO₂ formation. In the present study, this ratio τ is computed through the expression proposed by Campbell [3]:

$$\tau(t) = 10^{-\frac{2.1879 \times 10^3}{T_p(t)} + 2.3996}. \quad (4)$$

The global carbon conversion X_C is computed as the solution to the differential equation:

$$\frac{dX_C}{dt}(t) = \frac{R_C(t)}{m_C(0)}, \quad (5)$$

where $R_C(t)$ is the global carbon consumption rate at time t , which is expressed as:

$$R_C(t) = M_C k_s(t) \int_0^{R_p(t)} A_C(r, t) \rho_C(r, t) [O_2](r, t) r^2 dr, \quad (6)$$

M_C being the molar weight of carbon, k_s the kinetic constant for carbon combustion associated to the reaction (2) and which is given an Arrhenius expression, A_C the local specific surface area of the carbonaceous part, ρ_C the local apparent density of the carbonaceous part and $[O_2]$ the local oxygen concentration, the solution to the partial differential equation written in spherical coordinates:

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 D_{O_2}^e(r, t) \frac{\partial [O_2](r, t)}{\partial r} \right) = \frac{k_s(t) A_C(r, t) \rho_C(r, t) [O_2](r, t)}{\gamma(t)}, \quad (7)$$

following Hypothesis 4 concerning the preservation of the spherical symmetry of the particle. Here γ is the stoichiometric factor of the reaction of carbon combustion, $D_{O_2}^e$ the effective diffusivity of oxygen in the particle, k_d the oxygen mass transfer coefficient and $[O_2]_\infty$ the oxygen concentration at infinity, which is computed as: $[O_2]_\infty(t) = (P_{O_2})_\infty / (R_g T_g(t))$, with $(P_{O_2})_\infty = 0.12 \times 1.013 \times 10^5$ (Pa).

The following boundary condition at the surface of the particle:

$$\left(D_{O_2}^e \frac{\partial [O_2]}{\partial r} \right) (R_p, t) = k_d(t) ([O_2]_\infty(t) - [O_2](R_p, t)), \quad (8)$$

is imposed, together with the spherical symmetry condition at the center of the particle:

$$r^2 \left(D_{O_2}^e \frac{\partial [O_2]}{\partial r} \right) (r, t) \rightarrow_{r \rightarrow 0} 0. \quad (9)$$

The expression of the effective diffusivity of oxygen $D_{O_2}^e$ involves the Fick and Knudsen diffusion coefficients, see [10,11], for example. It thus takes into account the evolution of the particle structure versus time.

The instantaneous oxygen flux Φ_{O_2} at the particle surface is computed as:

$$\Phi_{O_2}(t) = k_d(t) 4\pi (R_p(t))^2 ([O_2]_\infty(t) - [O_2](R_p, t)). \quad (10)$$

Finally, the effectiveness factor η for the particle combustion is computed as:

$$\eta(t) = \frac{\Phi_{O_2}(t) \gamma(t)}{k_s(t) A_C(t) m_C(t) (1 - X_C(t)) [O_2](N_s(t), t)}. \quad (11)$$

Thermogravimetric experiments were performed to determine the kinetic constant k_s associated to the coal char combustion, which leads to the Arrhenius expression: $k_s(t) = 1050 \times \exp(-153,200 / (R_g T_p(t)))$, where R_g is the ideal gas constant. A great variety of pairs of kinetic parameters (pre-exponential factor and activation energy) may be observed in the literature for coal char combustion, [27].

2.5. Numerical Simulations of the Coal Char Combustion

In the combustion experiments performed on the coal char particles in the drop tube furnace, the initial time $t = 0$ s is chosen when the particle leaves the injection probe, which leads to the initial conditions: $T_p(0) = 323$ K, $X_C(0) = X_C(i, 0) = 0$ and $A_C(0) = A_C(i, 0) = 131,800 \text{ m}^2 \cdot \text{kg}^{-1}$. The other quantities which are involved in the present model start from the initial values indicated in Table 2.

Table 2. Initial values of the parameters involved in the model.

Experimentally Determined Values	Calculated Global Values	Local Values
$R_p(0) = 65 \times 10^{-6} \text{ (m)}$	$\rho_C(0) = 575.4 \times (1 - \tau_{ash}^0) = 434.4 \text{ (kg} \cdot \text{m}^{-3})$	$\rho_C(i, 0) = \rho_C(0) = 434.4 \text{ (kg} \cdot \text{m}^{-3})$
$\tau_{ash}^0 = 0.245$	$m_C(0) = \rho_C(0) \frac{4}{3} \pi (R_p(0))^3 \text{ (kg)}$	$\delta m_C(i, 0) = \rho_C(i, 0) \frac{4\pi}{3} (i^3 - (i-1)^3) dr^3 \text{ (kg)}$
$A_C(0) = 131,800 \text{ (m}^2 \cdot \text{kg}^{-1})$	$m_{ash}(0) = 575.4 \times \frac{4}{3} \pi (R_p(0))^3 \tau_{ash}^0$	$A_C(i, 0) = A_C(0) = 131,800 \text{ (m}^2 \cdot \text{kg}^{-1})$

$\delta m_C(i, 0)$ being the initial mass of carbon in the volume element i .

A Fortran code was written which numerically solves the problem (3), (7)–(9). A time step $dt = 2.0 \times 10^{-4}$ s was chosen. The progression with respect to the time parameter is obtained through the resolution of (3).

The key point of this Fortran code is the resolution of the problem (7)–(9), which is written in spherical coordinates, through a simple and efficient second-order finite difference method presented in [28]. In the present study, this finite difference method is adapted, evaluating the right-hand side member of (7) at the previous time step.

3. Results

The purpose of this section is to compare the results obtained through the numerical resolution of the model described in the preceding Section 2 and the experimental data (uniform particle temperature as measured by the two-color pyrometer). Figure 2 gathers the experimental and simulated particle temperatures for the three regulation temperatures of the drop tube furnace.

For the regulation temperature of 1100 °C, Figure 2a shows a very satisfying agreement between the experimental and simulated particle temperatures in the time range 0.25–0.86 s. In this time range, the difference between the maximal experimental (1246 °C) and simulated (1211 °C) temperatures is equal to 35 °C, which represents a relative difference of 2.8%. The times where the maximal temperatures are reached (0.425 s for the experimental curve and 0.404 s for the simulated curve) are very close, the relative difference being equal to 4.9%. The difference between the experimental and simulated temperature curves which is observed before $t = 0.25$ s is due to the fact that the initial condition $T_p(0) = 50$ °C is imposed in the model. The simulated particle temperature rapidly increases from this initial condition to 1050 °C which is reached at time $t = 0.25$ s. The two-color pyrometer measures a temperature slightly below 1100 °C inside the drop tube furnace.

For the regulation temperature of 1200 °C, Figure 2b also exhibits a very satisfying agreement between the experimental and simulated particle temperatures in the time range of 0.22–0.62 s. In this time range, the difference between the maximal experimental (1353 °C) and simulated (1386 °C) temperatures is equal to 33 °C, which represents a relative difference of 2.4%. The relative difference between the times corresponding to the maximal temperatures (0.342 s for the experimental curve and 0.310 s for the simulated curve) is equal to 9.4%.

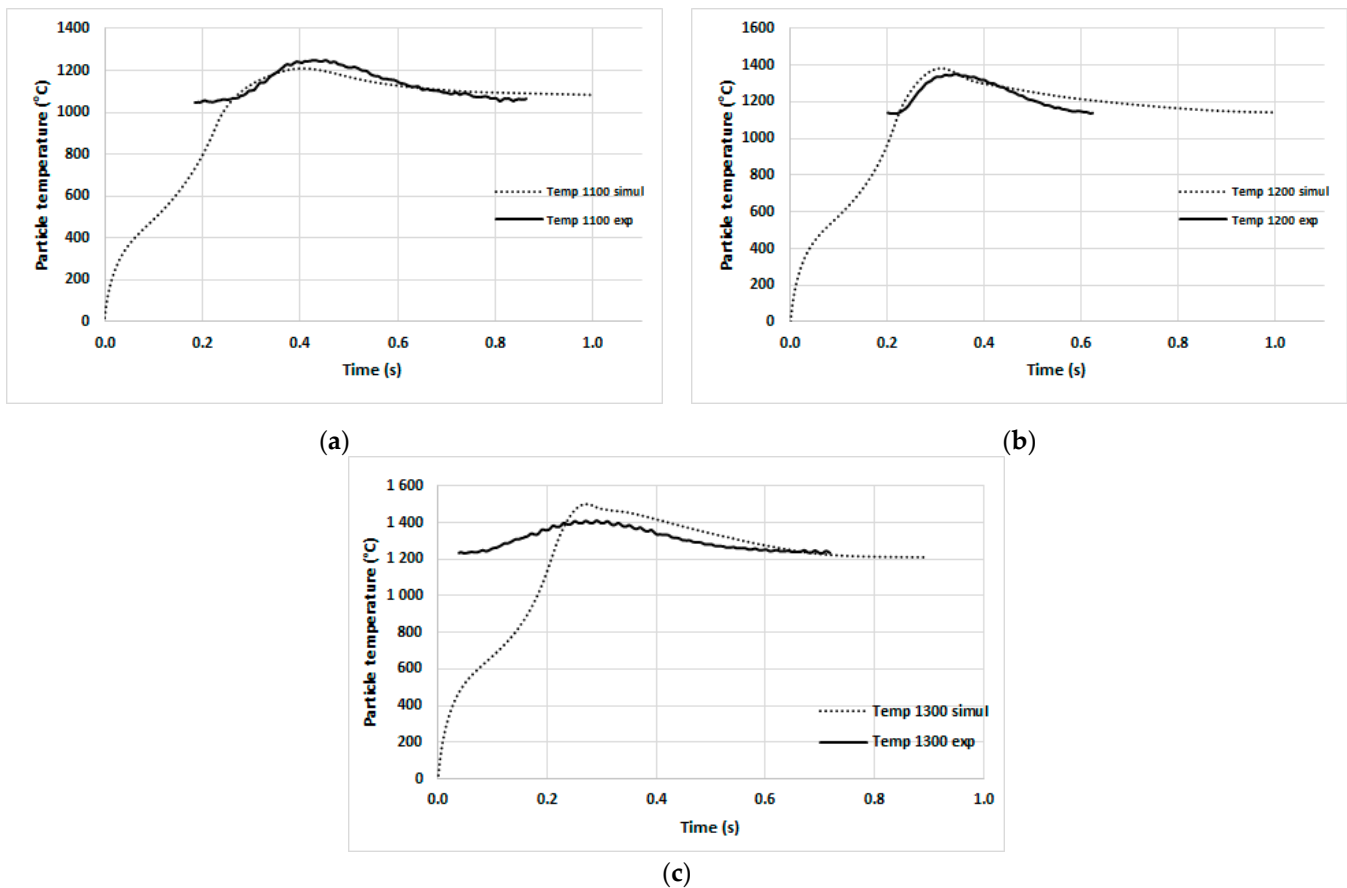


Figure 2. Experimental (solid line) and simulated (dotted line) particle temperature for the regulation temperature of the reactor equal to 1100 (a), 1200 (b) and 1300 °C (c).

For the regulation temperature of 1300 °C, Figure 2c, the experimental and simulated particle temperatures again well superimpose in the time range of 0.21–0.85 s. In this time range, the difference between the maximal experimental (1413 °C) and simulated (1505 °C) temperatures is equal to 91 °C, which represents a relative difference of 6.4%. The relative difference between the times corresponding to these maximal temperatures (0.290 s for the experimental curve and 0.271 s for the simulated curve) is equal to 6.6%. For this regulation of 1300 °C, the computations were stopped at 0.85 s, because the global carbon conversion was higher than 0.99 at that time. This means that at this “final” time, the carbon contained in the coal char particle has been almost totally removed from the particle.

When the regulation temperature increases from 1100 to 1200 and 1300 °C, the time at which the maximal experimental particle temperature is reached decreases from 0.425 to 0.342 and 0.290 s.

Figure 3 shows the evolution versus time of the global carbon conversion X_C , defined through the resolution of the differential Equation (5), of the effectiveness factor η_p , defined in (11) and of the normalized particle radius $R_p(t)/R_p(0)$, through the shrinking procedure exposed in Hypothesis 11, along the combustion experiment and for the three regulation temperatures of the reactor equal to 1100, 1200 and 1300 °C.

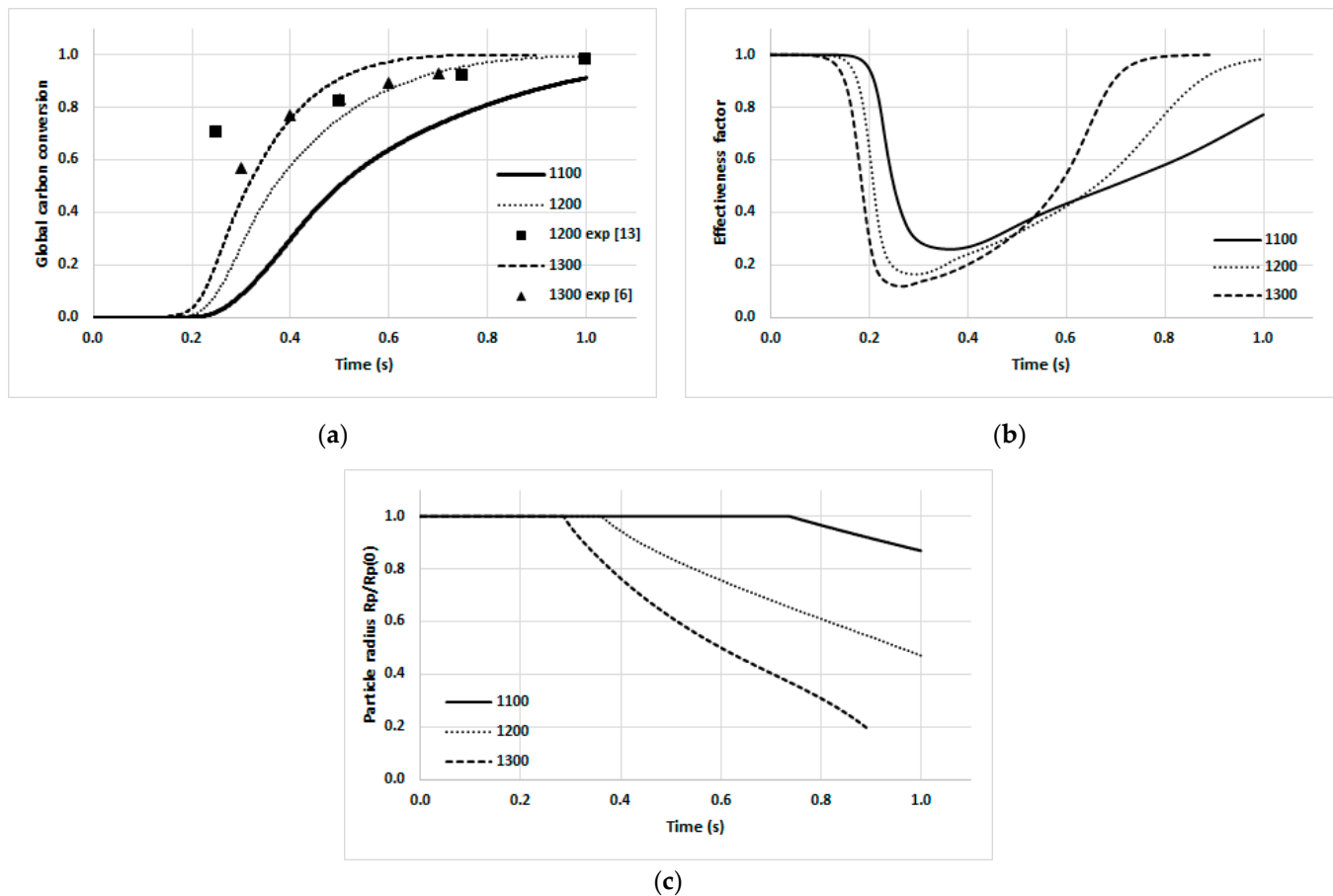


Figure 3. Global carbon conversion (a), effectiveness factor (b) and normalized radius of the coal char particle (c), during its combustion in the drop tube furnace, for the regulation temperature of 1100 (solid line), 1200 (dotted line) and 1300 °C (hyphenated line). The black squares and triangles in Figure 3a correspond to experimental data found in the literature, see the comments below.

As expected, the global carbon conversion increases faster when increasing the regulation temperature, Figure 3a. For the regulation temperature of 1100 °C, the global carbon conversion never reaches 1 in the time range of 0.0–1.0 s, Figure 3a (solid line). For the regulation temperature of 1200 °C, the global carbon conversion reaches 1 just before $t = 1$ s, Figure 3a (dotted line). For the regulation temperature of 1300 °C, the global carbon conversion reaches 1 at approximately $t = 0.75$ s, Figure 3a (hyphenated line). The four squares in Figure 3a correspond to the experimental values of the global carbon conversion obtained in [13], considering a furnace temperature of 1200 °C and an oxygen concentration of 5%, much lower than that (12%) considered in the present study. These experimental values of the carbon conversion are slightly different from that presented in the dotted line of Figure 3a, being over the simulated curve for the first value and below this simulated curve for the three other values. The five triangles of Figure 3a correspond to the experimental values of the global carbon conversion gathered from [6] (the triangle corresponding to $t = 0.5$ s being under the square). Here, the experiments were performed under the reactor temperature of 1300 °C and under an oxygen concentration of 20%, much higher than that of the present study. Again, these experimental points are slightly different from the simulated carbon conversions for this temperature, being slightly over the simulated curve for the first value and slightly below this simulated curve for the four other values. These differences may be explained by differences concerning the experimental conditions, as above-described, the coals used for the experiments and also the models leading to the simulated values. The authors here used a model combining a balance equation describing the evolution of the particle temperature that they solved using the iteration procedure

proposed in [29] and the computation of the effectiveness factor η through Equation (1) and a simple expression of the oxygen flux at the particle surface. In fact, the authors assumed a constant particle temperature, quoting from the literature that for particles with a size less than 100 μm , the variations in temperature do not significantly affect its combustion behavior. In [12], the authors compared the experimental and predicted values of the global carbon conversion, considering a furnace temperature of 1500 $^{\circ}\text{C}$ and an oxygen concentration of 21%. Under the minimal CO_2/Ar ratio of 5, the global carbon conversion was equal to 0.52 at $t = 0.20$ s, to 0.66 at $t = 0.25$ s, to 0.80 at $t = 0.30$ s and to 0.84 at $t = 0.40$ s. These values of the carbon conversion are higher than that presented in Figure 3a, but the furnace temperature was higher than the ones considered in the present study. The authors considered a spherical particle that they decomposed in hundreds of equally spaced concentric shells. They wrote an energy balance to compute the evolution of the particle temperature. They did not compute the oxygen concentration inside the particle, but they computed the effectiveness factor η through Equation (1) from Thiele modulus. In [10], the authors obtained a global carbon conversion approximately equal to 0.82 at time 1.3 s, when applying a regulation temperature of 1200 $^{\circ}\text{C}$ and an oxygen concentration of 21%. This is a much lower conversion than that observed in the present study for the same regulation temperature. One explanation for such a high difference could be the significant differences in the characteristics of the coals used for the experiments. Nevertheless, the simulations the authors obtained using CFD tools and the Thiele modulus method are in good agreement with their experimental conversions.

When changing the value of the particle radius with a variation of $\pm 20\%$, the maximal difference between the simulated global carbon conversions obtained for $R_p = 65$ μm and $R_p = 52$ μm is equal to 0.05, and that between the simulated conversions obtained for $R_p = 65$ μm and $R_p = 78$ μm is equal to 0.07. This proves that a variation of $\pm 20\%$ of the particle radius from the selected value (65 μm) does not significantly modify the simulations (relative difference of 5 and 7%, respectively).

The values of the effectiveness factor η_p defined in (11) exhibit a sharp decrease between 0.15 and 0.30 s, whatever the regulation temperature, Figure 3b, corresponding to a sharp increase of the particle temperature already observed in Figure 2. These low values of the effectiveness factor η_p prove the existence of high oxygen diffusion limitations, characteristic of zone II burning conditions. Even for the lowest regulation temperature of 1100 $^{\circ}\text{C}$, these diffusional limitations are present (η_p is less than 0.3 for times between 0.3 and 0.5 s).

Figure 3c shows that the normalized particle radius $R_p(t)/R_p(0)$ regularly decreases after the removal of the first outer volume element which occurs at times 0.73, 0.36 or 0.29 s, in the case of a regulation temperature equal to 1100, 1200 or 1300 $^{\circ}\text{C}$, respectively. In the case of the regulation temperature of 1100, 1200 or 1300 $^{\circ}\text{C}$, the number of volume elements decreases to 434, 235 or less than 94, respectively. As previously discussed, the computations were stopped at $t = 0.85$ s for the regulation temperature of 1300 $^{\circ}\text{C}$, because the global carbon conversion X_C was higher than 0.99, Figure 3a, although the particle radius was not equal to 0 at this final time, Figure 3c. As the volume elements have the size thickness, they contain less carbon when they are close to the center of the particle.

4. Discussion

The model which is proposed in the present study also gives access to local quantities and their variations within the coal char particle during its combustion. To better understand how the combustion evolves within the particle, the behavior of different local quantities is analyzed here during the combustion process. The local oxygen concentration $[\text{O}_2](i,.) (\text{mol.m}^{-3})$ and the product $(A_C \rho_C)(i,.) (\text{m}^2.\text{m}^{-3})$ between the local carbonaceous material density $\rho_C(i,.) (\text{kg.m}^{-3})$ and the local specific area $A_C(i,.)$, which is the area of the reactive carbon surface per volume unit, are the key parameters for the combustion

rates. These local quantities allow the local carbon consumption rate per volume unit $r_c(i,.)$ ($\text{kg.s}^{-1}.\text{m}^{-3}$) to be analyzed, given through:

$$r_c(r, t) = M_C k_s(t) A_C(r, t) \rho_C(r, t) [O_2](r, t) \quad (12)$$

and to the local carbon conversion $X_C(i,.)$ computed through:

$$X_C(r, t + dt) = X_C(r, t) + M_C k_s(t) A_C(r, t) [O_2](r, t) (1 - X_C(r, t)) dt. \quad (13)$$

Six times $(t_j)_{j=1,\dots,6}$ are chosen along the combustion process to analyze the behavior of the above-indicated local quantities within the particle. Their values, together with that of the corresponding global carbon conversion, particle temperature, particle radius and label of the outer volume element, returned for a regulation temperature of the reactor equal to 1200 °C, are gathered in Table 3. These six chosen times are sufficient to analyze the trends of the different local quantities previously indicated, whence the combustion behavior of the particle.

Table 3. Calculated quantities at six times of the combustion of a coal char particle in the drop tube furnace. Regulation temperature: 1200 °C.

Time t_j (s)	0.256	0.284	0.320	0.357	0.424	0.569
Global carbon conversion $X_C(t_j)$	0.11	0.21	0.35	0.47	0.63	0.84
Particle temperature $T_p(t_j)$ (°C)	1292	1364	1382	1339	1291	1228
Particle radius $R_p(t_j)$ (µm)	65.0	65.0	65.0	65.0	59.4	50.8
Outer volume number $N_s(t_j)$	500	500	500	500	457	391

Figure 4 presents the values of the local carbon conversion, oxygen concentration, relative surface per unit volume and carbon consumption rates at the six chosen times indicated in Table 3, in terms of the volume element number and computed according to Equations (12) and (13).

The curves of the different local quantities present quite the same shape for the six chosen times, being mainly translated.

Looking at the local carbon conversion curves and especially at the right extremities of the four curves corresponding to the four lower chosen times of 0.256, 0.284, 0.320 and 0.357 s, Figure 4a, the outer element volume exhibits a local carbon conversion ranging from 0.4 to approximately 1. This is because this outer volume element is progressively consumed and close to disappearing. The local carbon conversions drastically decrease from the right extremity (which corresponds to the number of the surface volume element) toward the particle center, up to the left extremity of the curve where the local carbon conversions are equal to 0. The distance between these two extremities on the horizontal axis defines the zone of the particle where the combustion is active at time t . The combustion is more active close to the particle surface and decreases down to 0 at the left extremity of the curve (center of the particle). At every chosen time t_j , only a spherical shell (containing roughly 150 volume elements) is burning under a significant oxygen concentration. The thickness of the combustion zone in which combustion occurs at a given time does not highly vary, while this zone progresses toward the particle center. It mainly occurs at the particle surface due to the particle shrinking. Just a small broadening is observed. This is in relation with the decrease of the particle radius and the increase of the porosity which makes the oxygen diffusion more efficient in a neighborhood of the particle surface.

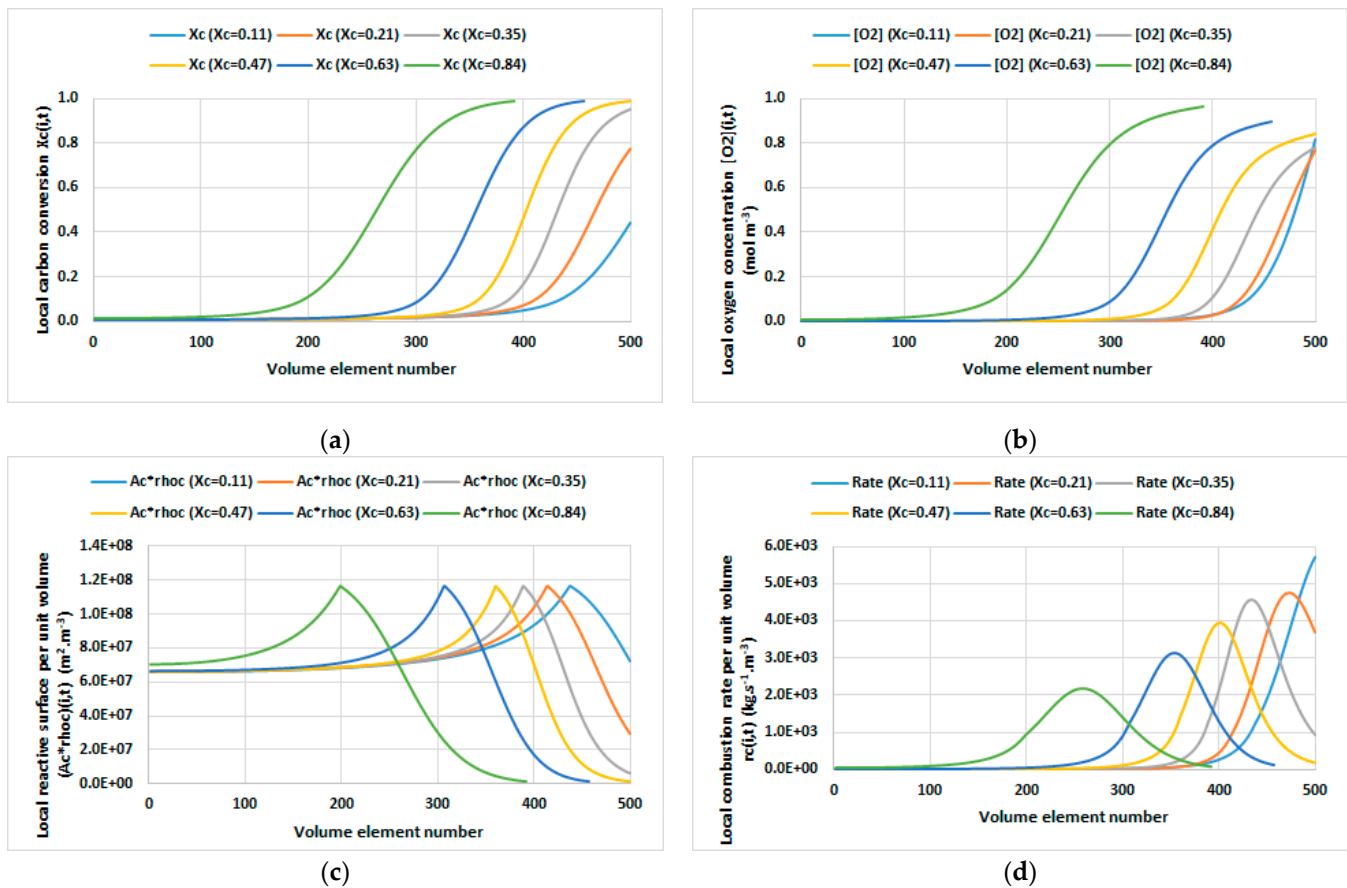


Figure 4. Local carbon conversions X_c (a), oxygen concentrations $[O_2]$ (b), local reactive surface per unit volume $A_c \rho_c$, (c), and local carbon consumption rates r_c (d), at the six chosen times indicated in Table 3, and for the regulation temperature of the reactor equal to 1200 °C.

The oxygen concentration curves, Figure 4b, are in complete agreement with the local carbon conversion ones. The four curves corresponding to the four first times end at the particle surface with close but different oxygen concentrations, due to the evolution of the particle temperature with respect to time. These curves are in agreement with the values of the efficiency factor η_p above-discussed, confirming that the combustion is controlled by both diffusion and kinetics of combustion.

Figure 4c shows the variations of the local value of the product $(A_c \rho_c)(i, .)$, which represents the area of the carbon surface available for combustion per volume unit, versus the number of the volume element. In a given volume element, the local product $(A_c \rho_c)(i, .)$ increases from its initial value, according to the increase of the specific surface area A_c up to its maximum 300,000 $m^2 \cdot kg^{-1}$ and the decrease of the carbon density ρ_c due to the local consumption of carbon, while the specific surface area A_c is forced to stay at its maximum. Every volume element undergoes a very similar variation. The maxima of this product are identical for all volume elements because the specific surface area A_c reaches the same maximum corresponding to the same limit (300,000 $m^2 \cdot kg^{-1}$) for the same local carbon conversion ($X_c = 0.11$). After this maximum, the decrease of the carbon density ρ_c controls the decrease of the product $A_c \rho_c$ until the end of this local combustion. During the combustion propagation, this process is successively followed by every volume element, but at different times and with different durations due to the temperature variations. This explains the succession of widening peaks along the radius, whose amplitude is limited by the same maxima. The two first curves ($t = 0.256$ and 0.284 s) present a particular shape because at those times, the outer element number 500 already started to evolve.

Figure 4d shows the variations of the local combustion rate r_C per volume unit, defined in (11). The local combustion rate contains the kinetic constant k_s which only depends on the temperature, the local product $(A_C \rho_C)(i, .)$ and the local oxygen concentration $[O_2](i, .)$. The variations of the local combustion rate versus the volume element combine the effects of the variations of these quantities. They also exhibit successive peaks but with a curved decreasing maximum when the element number i decreases. This is explained by the decrease of the oxygen concentration when the combustion front moves toward the particle center and by the decrease of the particle temperature when the combustion zone reaches the elements with numbers less than 300.

Instead of Campbell's expression (4) of the ratio τ between the instantaneous rates of CO and CO₂ formation, that of Laurendeau could be used, [3], which is defined as:

$$\tau(t) = 10^{2.5} \exp\left(-\frac{25,000}{R_g T_p(t)}\right). \quad (14)$$

The impact of the expression of the ratio τ on the radiation, convection and enthalpy terms in the right-hand side of Equation (3) is analyzed in Figure 5.

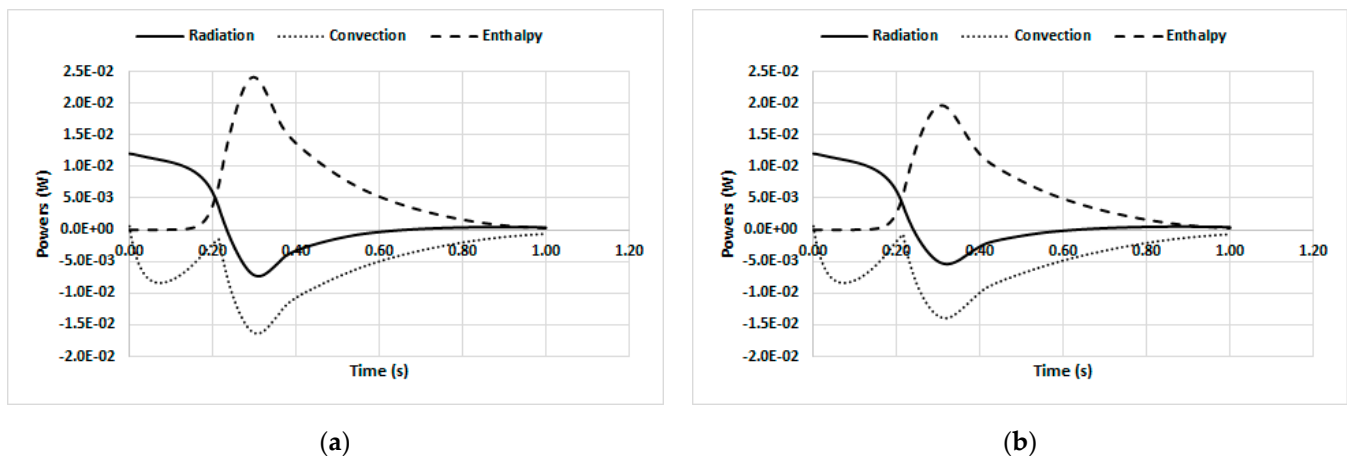


Figure 5. Values of the radiation (solid line), convection (dotted line) and enthalpy (hyphenated line) terms in the right-hand side of (3) versus time, according to Campbell's (a) and Laurendeau's (b) equations, and for the regulation temperature of the reactor equal to 1200 °C.

During particle combustion which occurs between 0.2 and 0.8 s, most of the energy is exchanged by the particle through the enthalpy of the reaction, the hyphenated line, according to the area lying between the enthalpy curve and the time axis. This exchange contributes to approximately 50% of the total exchanged energy (absolute values considered). The maximum of the enthalpy power (which contains the ratio τ) increases from 1.97×10^{-2} W with Laurendeau's equation (at 0.298 s) to 2.41×10^{-2} W with Campbell's equation (at 0.307 s), corresponding to a 22% increase. This result is in agreement with the drastic decrease of the ratio τ when changing Laurendeau's equation to Campbell's one. For the radiative power, the effect is more pronounced with an increase from 5.41×10^{-3} to 7.32×10^{-3} W, representing a 35% increase, when passing from Laurendeau's to Campbell's equations. The convective power increases from 1.39×10^{-2} to 1.64×10^{-2} W, representing a 18% increase. The radiative power is more affected than the two others by the change of equation for τ because of the temperature dependence in T^4 .

To conclude this Discussion section, a comparison is established between the results of the present study which considers a shrinking coal particle and that of the previous study [20] which considered a coal char particle with a fixed radius along the combustion process. Laurendeau's equation (14) of the ratio τ between the instantaneous CO and CO₂ formation rates was used in the previous study [20]. Consequently, the simulations are also performed with the present model involving Laurendeau's equation. The particle

temperature and the global carbon conversion obtained with the two models are compared in Figure 6, for the regulation temperature of the reactor equal to 1200 °C.

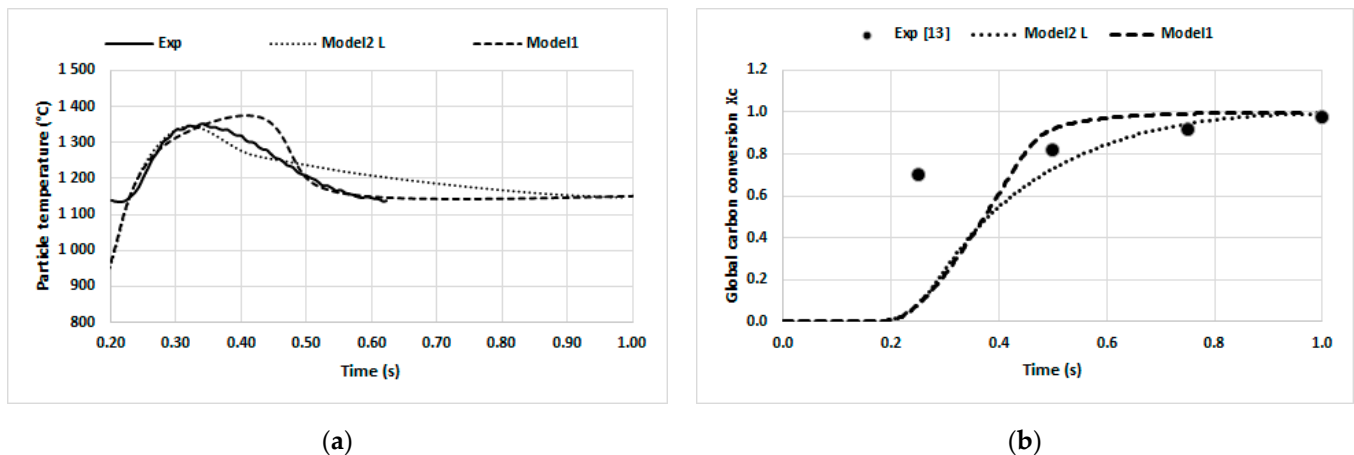


Figure 6. Comparison of the particle temperature (a) and of the global carbon conversion (b), returned by the present model (called Model2 L, dotted line) with Laurendeau’s equation and the previous model (called Modell, hyphenated line). The experimental particle temperature is represented with a solid line in Figure 6a. The black points in Figure 6b correspond to experimental values taken from [13]. Regulation temperature of the reactor equal to 1200 °C.

The curves of Figure 6a are presented in the time range 0.2–1.0 s, to highlight the active combustion time range, as previously discussed. The maximal particle temperatures returned by the two models show an acceptable agreement (difference approximately equal to 31 °C) between both models, but the difference between the times at which these maxima are reached is significantly high (0.09 s), Figure 6a. The maximal differences between the simulated and experimental particle temperatures are quite the same (approximately 70 °C). They are higher than that obtained when considering Campbell’s Equation (4) for the ratio τ . In the time range 0.25–0.60 s, the shape of the curve presenting the particle temperature simulated through Model 2 L with Laurendeau’s equation is closer to that of the experimental temperature than that returned by Model 1.

The comparison of the two global carbon conversions shows a significant difference, Figure 6b. The simulated carbon conversion curve obtained with Model 2 L is always higher than that obtained with the previous model. The first experimental point indicated in [13] (time equal to 0.25 s) is largely above the two simulated curves. The second experimental point (time equal to 0.5 s) lies between the two curves. The last two experimental points are closer to the simulated curve obtained when considering the present model than the previous one. It is however difficult to conclude from these four observations, further observing that the four experimental values were obtained under slightly different experimental conditions than that of the present study.

Similar observations can be brought for the two other regulation temperatures of the reactor.

5. Conclusions

A simple model was proposed which simulates the combustion of a pulverized coal char particle falling in a drop tube furnace. The particle was allowed to shrink during its fall, but kept its spherical symmetry. For three regulation temperatures of the reactor (1100, 1200 and 1300 °C), the particle temperatures calculated by the model were in good agreement with the experimental ones measured by a two-color pyrometer. Local quantities (oxygen concentration, particle density, carbon conversion, specific surface area and combustion rate) were computed along the particle radius and during the combustion process. The effectiveness factor of the particle was calculated during the combustion process. The

values returned by the model together with the computed local quantities are in agreement with a zone II combustion, with high oxygen gradients prevailing along the particle radius, generating the development of the non-uniform structure and the shrinking of the spherical particle during its combustion. Even within such a small particle, the presence of a very abrupt combustion front and the shrinking of the particle justify to account for the gradients of different local quantities along the particle radius during the combustion process. Even if the model which is proposed is based on simplifying the hypotheses (mainly preservation of the spherical geometry of the particle and uniformity of the temperature within the particle), the simulations are in good agreement with the experimental data and with the results of the literature. To achieve more complete agreement between the experiments and simulations in the present context, improvements should be performed both on the measurements of the temperature and of the particle mass during its fall in the drop tube furnace.

Although the present study is limited to simulations of the combustion of a coal char particle in a drop tube furnace, the combustion of other feedstock could be simulated with the proposed model with slight modifications concerning the characteristics of the feedstock.

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Nomenclature

A_C	specific surface area of char, $\text{m}^2.\text{kg}^{-1}$	R_C	combustion rate, $\text{kg}.\text{s}^{-1}.\text{m}^{-3}$
$C_{p,C}$	calorific capacity of carbon, $\text{J}.\text{kg}^{-1}.\text{K}^{-1}$	R_p	particle radius, m
$C_{p,ash}$	calorific capacity of ash, $\text{J}.\text{kg}^{-1}.\text{K}^{-1}$	R_r	reactor radius, m
dr	thickness of each volume element of the particle, m	T_g	gas temperature, K
dt	time step, s	T_p	particle temperature, K
$D_{O_2}^e$	effective diffusivity of oxygen within the particle, $\text{m}^2.\text{s}^{-1}$	T_{wall}	wall temperature, K
F_g^0	gas flow at 298 K, $\text{m}^3.\text{s}^{-1}$	u_g	gas velocity, $\text{m}.\text{s}^{-1}$
h	convective heat transfer coefficient, $\text{W}.\text{m}^{-2}.\text{K}^{-1}$	X_C	carbon conversion

i	volume element number	γ	molar stoichiometric factor, $\text{mol}_C \cdot (\text{mol}_{O_2})^{-1}$
k_s	kinetic constant, $\text{m} \cdot \text{s}^{-1}$	δm_C	elementary carbon mass within a volume element, kg
m_C	carbon mass within the char particle, kg	$\Delta_R H_{CO}^0$	reaction enthalpy for CO formation, $\text{J} \cdot \text{mol}^{-1}$
m_{ash}	total ash mass within the particle, kg	$\Delta_R H_{CO_2}^0$	reaction enthalpy for CO_2 formation, $\text{J} \cdot \text{mol}^{-1}$
N	number of concentric volume elements	ε_p	char particle emissivity
N_s	number of the outer volume element	Φ_{O_2}	molar oxygen flux, $\text{mol} \cdot \text{s}^{-1}$
$[O_2]$	oxygen concentration within the char particle, $\text{mol} \cdot \text{m}^{-3}$	η	particle effectiveness factor
$[O_2]_\infty$	oxygen concentration far from the particle, $\text{mol} \cdot \text{m}^{-3}$	Φ	Thiele modulus
P_{O_2}	pressure, Pa	ρ_C	apparent density of carbonaceous particle material, $\text{kg} \cdot \text{m}^{-3}$
r_c	local combustion rate $\text{kg} \cdot \text{s}^{-1} \cdot \text{m}^{-3}$	σ	Stefan-Boltzmann constant, $\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-4}$
		τ	molar ratio CO/CO_2

Some quantities such as A_C or X_C

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