THEORETICAL ANALYSIS OF HEAT TRANSFER IN A PULVERIZED COAL COMBUSTION CHAMBER UNDER O_2/CO_2 ATMOSPHERE

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Abstract.

Oxy-fuel combustion is a promising technique in the technology of recovering CO_2 from flue gas generated by coal-fired power plants. The fuel in this technology is burned in an O_2/CO_2 mixture instead of air, raising the CO_2 concentration in the flue gas to provide easy sequestration. It is known that the combustion behavior, pollutant emissions and heat transfer characteristics in such atmospheres could differ considerably with air combustion depending on O_2 concentration. In order to better understanding the characteristics of pulverized coal combustion in such atmospheres, numerical simulations of an available case in the literature are performed using a CFD code. Basically, the mathematical model is based on a Eulerian description for the continuum phase and a stochastic Lagrangian description for the coal particles. In this work, different parameter comparison related to heat transfer characteristics in air and in O_2/CO_2 atmospheres are presented.

Keywords*: Oxy-fuel technology, pulverized coal combustion, oxy-fuel numerical modeling.*

1. INTRODUCTION

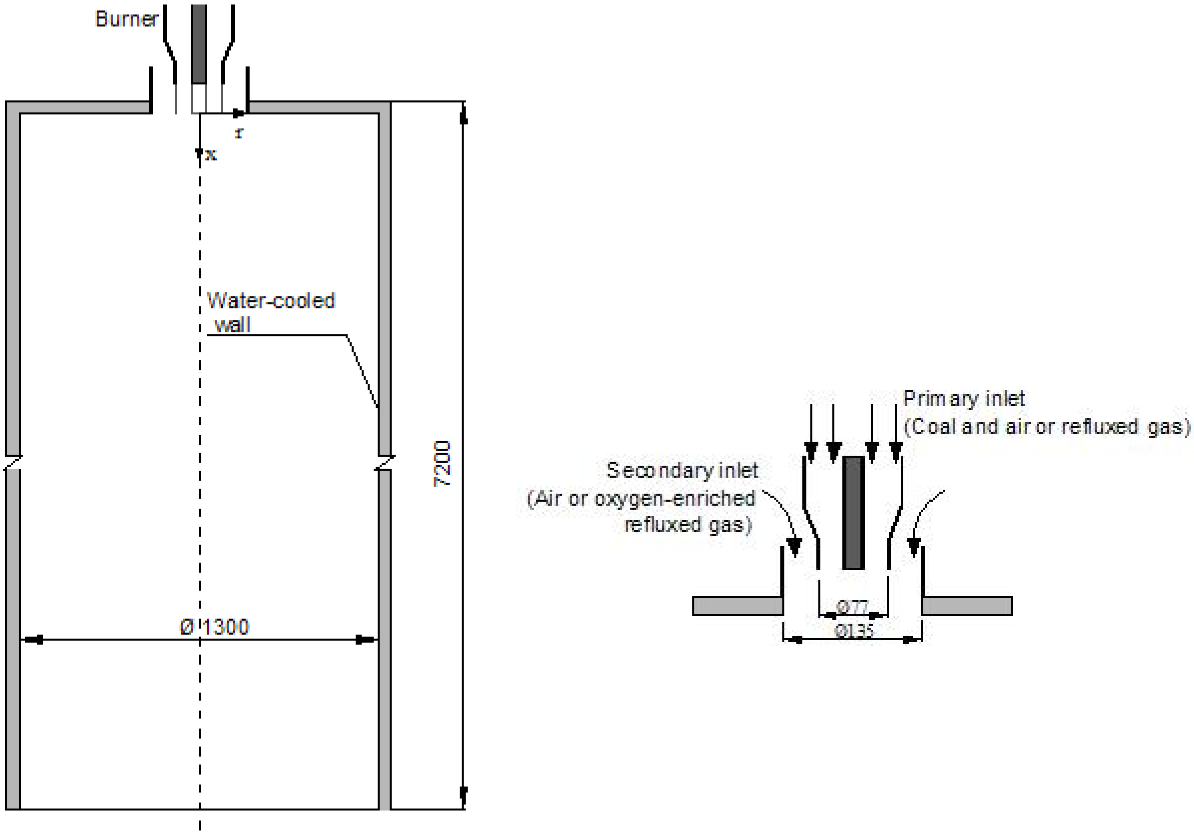
Global coal use is growing significantly due to its wide availability, stability of supply and cost. According to the International Energy Agency's World Energy Outlook 2004, it is projected that by 2030 coal will account for around 22% of the world energy mix. Although in recent years have seen a significant pressure on coal-fired power stations to limit pollutant emissions, it is expected that coal will continue to play a significant role in power generation. However, to maintain its position in the global energy mix, technological solutions for reducing greenhouse gas emissions become an important issue. Among the possible technologies for emissions control from coal-fired power generation, CO_2 capture and storage has been recognized as a promising option for achieving significant results. This offers the prospect of a power plant with near-zero emissions of CO_2.

In a general way, the main purpose of CO_2 capture is to produce a concentrated stream of CO_2 at high pressure that can readily be transported to a storage site in secure geological formations. Although the entire gas stream containing low concentrations of CO_2 could be transported and stored underground, the high associated costs make such method impractical (Minchener and McMullan, 2007). The concept of CO_2 capture and storage is usually divided into three approaches, namely post-combustion capture, pre-combustion capture, and oxy-fuel techniques. The current work is focused on the oxy-fuel option especially on pulverized coal systems.

During the oxy-fuel combustion, a combination of oxygen typically of greater than 95% purity and recycled flue gas are used for combustion of the fuel instead of air. According to Buhre *et.al.* (2005), by recycling the flue gas, a gas consisting mainly of CO_2 and water is generated, ready for sequestration without stripping of the CO_2 from the gas stream. Besides, the recycled flue gas is used to control flame temperature and make up the volume of the missing N_2 to ensure there is enough gas to keep an approximated heat transfer in the convective section of the boiler. It is known that the combustion behavior, pollutant emissions and heat transfer characteristics in such atmospheres could differ considerably with air combustion depending on O_2 concentration. Through a theoretical approach, the goal of this paper is to evaluate the heat transfer characteristics inside a pulverized coal combustion chamber in air and in O_2/CO_2 atmospheres. In order to obtain first results, a pioneer work available in the literature was chosen as reference to perform numerical simulations using a CFD code.

2. DESCRIPTION OF THE PROBLEM

It is considered the test cases investigated by Khare *et.al.*(2008). The combustion system is a cylindrical and down-fired vertical combustor (1.3 m diameter and 7.2 m long). It has a rated firing of up to 1.2 MW_{th} capable of operating under air-fired and oxy-fuel conditions. The furnace is refractory lined and a water-cooling jacket in the outer wall. A swirl pulverized coal burner is installed at the top of the furnace and its geometry can be observed in Figure 1 (b). The coal utilized is classified as sub-bituminous and the operational conditions are also detailed in the Table 1. In the oxy-fuel case, the flue gas is recirculated to the primary and secondary inlets and only the secondary is enriched with 0.3 O_2 volume concentration.



(a) (b)

Figure 1 – Geometry of the combustion chamber and burner. Adapted from Khare *et.al.*(2008).

Table 1. Furnace operating conditions. Adapted from Khare *et.al.*(2008).

Inlet conditions	Air-fired	Oxy-fuel
Thermal power (MW_{th})	0.80	0.80
Coal feed rate (kg/h)	120	120
Primary air /refluxed gas (kg/h)	195	240
Primary velocity (m/s)	20	23
Primary swirl number	0	0
Primary temperature (K)	353	403
Secondary air / refluxed gas (kg/h)	780	625
Secondary velocity (m/s)	35	21
Secondary swirl number	0.20	0.20
Secondary temperature (K)	553	493

3. NUMERICAL MODELING

3.1 Governing equations

The mathematical model is based on a commercial CFD code (FLUENT 6.3.26) through an Euler-Lagrange approach. The fluid phase is treated as a continuum by solving the time-averaged equations of global mass, momentum, enthalpy and species mass fractions, while the dispersed phase is solved by tracking a large number of particles through the calculated flow field. The general form of the gas-phase equations for axisymmetric turbulent flow in a cylindrical geometry is described by Eq. (1).

$$\frac{\partial(\rho u\phi)}{\partial x}+\frac{1}{\rho}\frac{\partial(r\rho v\phi)}{\partial r}=\frac{\partial}{\partial x}\left(\Gamma_\phi\frac{\partial\phi}{\partial x}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left(r\Gamma_\phi\frac{\partial\phi}{\partial r}\right)+S_\phi \tag{1}$$

The generic variable, ϕ, represents an unitary value for the conservation of mass and u, v and w for axial-, radial- and tangential-momentum. In the case of conservation equations for species and energy, ϕ becomes the mass fraction and enthalpy, respectively. The turbulence effects are here modeled using the widely used standard k-ε, where in above equation ϕ represents k for turbulent kinetic energy and ε for the energy dissipation rate. Although the k-ε model does not predict good results in some cases, for pulverized-coal systems without high swirl effects, this model could be considered the most practical choice (Smoot and Smith, 1985).

For the reaction chemistry, the coal combustion is modeled using the non-premixed approach. In this model, the combustion is simplified to a mixing problem, and the difficulties associated with closing non-linear mean reactions rates are avoided. Besides, the model provides a better computational efficiency because it does not require the solution of a large number of species transport equations (Fluent, 2006). Basically, the basis of the non-premixed modeling is that under a certain set of simplifying assumptions, as for instance chemical equilibrium, the thermochemical scalars (species fractions, density, and temperature) are related to one or two conserved scalar quantity known as the mixture fractions. The conservation equation for the new scalar also have the form of the Eq.(1), where ϕ represents a mean mixture fraction. In addition, a conservation equation for the mixture fraction variance is also solved. To the air-fired case one conserved mixture fraction equation is computed while in the oxy-fuel case, two mixture fractions are necessary. During the solution procedure, the information about thermo-chemistry and its interaction with turbulence are obtained from the probabilistic density function (PDF) database. A table is calculated before running the simulation and contains time-averaged values of temperature, composition, and density at discrete values of mixture-fraction and mixture fraction variance.

The particles of coal dispersed in the continuous phase are modeled through different models following a Lagrange approach. The spherical particle distribution is modeled using a Rosin-Rammler method. A particle range size between 1 and 200 μm diameter and a mean of 60 μm diameter are utilized. The trajectory of a discrete particle is predicted by integrating the force balance on the particle (Fluent, 2006). Such balance equates the particle inertia with the forces acting on the particle according to Eq. (2) where the terms of the right hand refer to the drag force, gravity and additional forces, respectively. Besides, the dispersion of particles due to turbulence in the fluid is predicted using the stochastic tracking (randon walk) model.

$$\frac{du_P}{dt}=F_D(u-u_P)+\frac{g_x(\rho_P-\rho)}{\rho_P}+F_x \tag{2}$$

The volatile evolution and char combustion are modeled using different steps according to involved phenomena. While the particle does not reach the vaporization temperature, a simple heat balance is applied to calculate the particle temperature as given by Eq.(3). The same heat balance is applied also after the combustible fraction has been consumed since a particle may contain residual ash.

$$m_P c_P\frac{dT_P}{dt}=hA_P(T_\infty-T_P)+\varepsilon_P A_P\sigma\left(T_R{}^4-T_P{}^4\right) \tag{3}$$

A devolatilization model is applied to the combusting particle when its temperature reaches the vaporization level and remains in effect while the mass of the particle exceeds the mass of the nonvolatiles in the particle. A single kinetic rate devolatilization model is utilized. Such model assumes that the rate of devolatilization is first-order dependent on the amount of volatiles remaining in the particle according to Eq. (4) (Bazioch and Hawksley, 1970). The kinetic rate, k, is defined by input of an Arrhenius type pre-exponential factor and an activation energy.

$$-\frac{dm_P}{dt} = k\left[m_P - \left(1 - f_{v,0}\right)\left(1 - f_{w,0}\right)m_{P,0}\right] \tag{4}$$

After the volatiles are completely evolved, a surface reaction begins which consumes all the combustible fraction of the particle. The kinetic/diffusion-limited rate model is applied in the simulations, which assumes that the surface reaction rate is determined either by kinetic or by a diffusion rate (Fluent, 2006). The diffusion rate coefficient, reaction rate and the char combustion rate are described in the Eq. (5), (6) and (7), respectively. The input parameters to the devolatilization and char combustion models are related by Khare *et.al.*(2008).

$$D_0 = \frac{C_1\left[\left(T_P + T_\infty\right)/2\right]^{0,75}}{d_P} \tag{5}$$

$$\Re = C_2 e^{-\left(E/RT_P\right)} \tag{6}$$

$$\frac{dm_P}{dt} = -A_P p_{OX} \frac{D_0 \Re}{D_0 + \Re} \tag{7}$$

The radiation has an important issue inside furnaces and the accuracy of its calculation depends on a combination of an adequate solution method and the accuracy to which the properties of the radiating media and surrounding walls are known. The general form of the radiative transfer equation for an absorbing, emitting, and scattering medium is described by Eq. (8). This differential equation is solved by using P-1 model, which is based on the expansion of the radiation intensity I into an orthogonal series of spherical harmonics (Siegel and Howell, 2002). The weighted-sum-of-gray-gases (WSGGM) has been defined for computation of the absorption coefficient.

$$\frac{dI}{ds} + \left(a + \sigma_S\right)I = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_S}{4\pi}\int_0^{4\pi} I.\Phi \, d\Omega' \tag{8}$$

3.2 Numerical details

The computations are performed on a two-dimensional grid with higher concentration of quadrilateral elements in the near burner region. It is important to consider that a mesh quality is critical for a good convergence and accuracy in such problems. Thus, several parameters have been adopted to ensure a good mesh quality, as for instance: low skewness, moderate aspect ratios, smooth change in the mesh size, and orthogonality at boundaries. Different mesh refinements were also created to perform a grid independence analysis. The number of elements of testing meshes is 18000, 42120 and 139323.

Besides the boundary conditions already summarized in the Table 1 another inputs are necessary. Turbulence boundary conditions are determined based on 10% turbulent intensity and hydraulic diameters of primary and secondary inlets (Table 3). Also, it is assumed that the combustion chamber walls are maintained at the temperature of 1200 K, in addition to the non-slip and impermeability conditions.

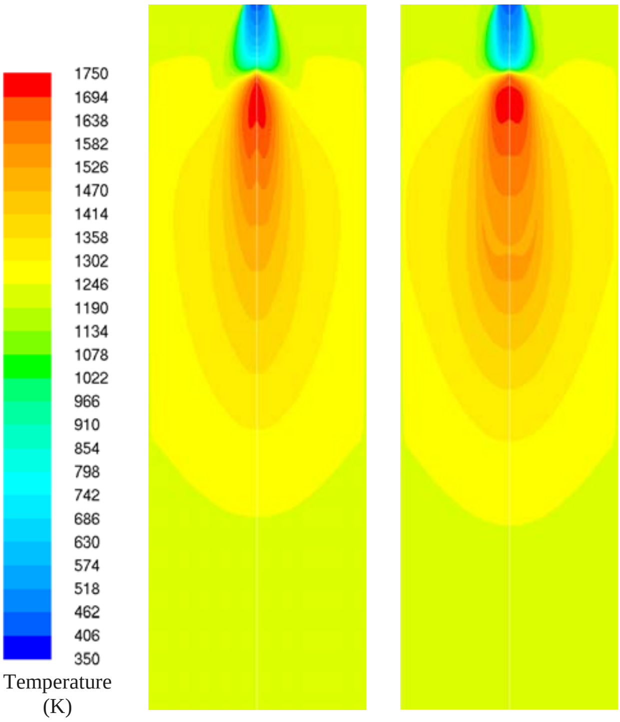
Table 3. Turbulence boundary conditions.

		Air-fired	Oxy-fuel
Primary inlet	k turbulent kinetic energy (m^2/s^2)	40	52.90
	ε energy dissipation rate (m^2/s^3)	818.29	1244.52
Secondary inlet	k turbulent kinetic energy (m^2/s^2)	122.50	44.10
	ε energy dissipation rate (m^2/s^3)	2627.18	567.47

The advective terms of momentum, energy, and mean mixture fraction equations are discretized through a second order upwind scheme, while the terms related to pressure, are discretized using the PRESTO scheme. The set of discretized equations is solved through a segregate approach and the pressure-velocity coupling is treated by using the SIMPLE method. The solution process is initially carried out without involving reactions and discrete phase coal particles and then once the convergence is achieved, simulation is continued involving coal particles. After the convergence of all equations, the last step is to insert the radiation model in the iterative process. The solution has been assumed ρρ converged when the residual are less than 10^{-3} except for energy, radiation and mixture fraction, which are considered satisfactory less than 10^{-6}. Monitoring points have been also defined at the symmetry line to verify the stability of different variables along the iterations.

5. RESULTS AND DISCUSSION

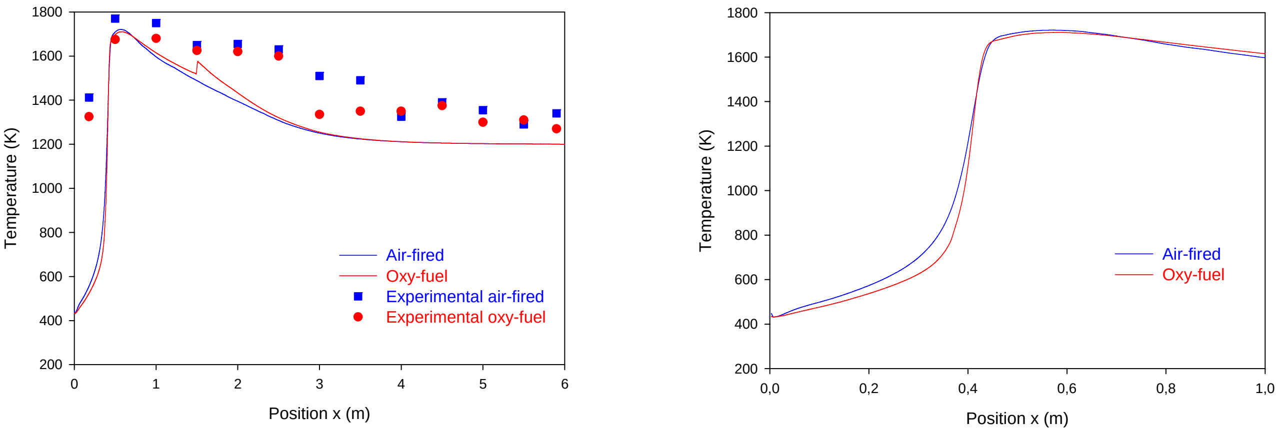
Figure 2 shows the temperature distribution inside the combustion chamber to air-fired and oxy-fuel case in the first 4 meters. As expected, due to the low swirl number, a central flame without reaching the walls is obtained to both cases. Although the oxy-fuel flame has been larger, a similar flame shape and approximated temperature levels can be observed within combustion chamber to both cases.



(a) Air-fired case (b) Oxy-fuel case

Figure 2 – Temperature distribution inside the combustion chamber.

Temperature profiles at center line are presented in the Figure 3 (a) and (b) and a good accordance with experimental results may be verified. A very small delaying ignition is observed in the oxy-fuel case. According to Kiga *et.al.* (1997), due to small difference of thermal conductivity of each gas mixture, the difference in specific heat could be pointed a reason for slower flame propagation speed in the O_2/CO_2 atmospheres. The average thermal conductivity to both cases is approximately 0.08 W/mK and the average specific heat to air-fired and oxy-fuel case is 1262 J/kgK and 1340 J/kgK, respectively.

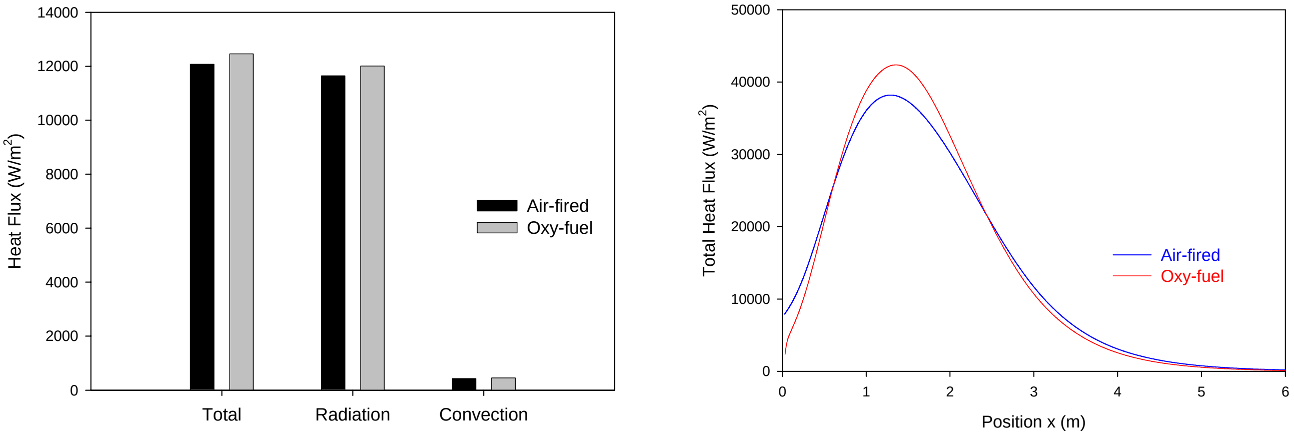


(a) (b)

Figure 3 – Temperature along the furnace center line. Experimental results available in Khare *et. al.* (2008).

Figure 4 (a) compares the heat transfer modes and Figure 4 (b) shows heat flux distribution at lateral wall. Although it is observed a similar profile, higher values are obtained in the oxy-fuel case. The average total heat flux to the air-fired and oxy-fuel case are 12072 W/m² and 12458 W/m², respectively. The oxidant mass flow in the oxy-fuel case is reduced by about 11.3% and the density increased from 0.3 kg/m³ to 0.4 kg/m³ due to higher concentration of CO_2 which holds a molecular weight higher than N_2. Thus, the average heat transfer coefficient at wall is increased from 8.6 W/m²K (air-fired case) to 13.6 W/m²K (oxy-fuel case) that explains a lower convection heat flux in the air-fired case (429 W/m²) when compared to the oxy-fuel case (452 W/m²).

It is also well-known radiation plays an important role inside combustion chambers and a special attention must be given to the combustion process in oxy-fuel atmospheres, where the presence of polar gases is increased significantly. By recycling flue gas, the presence of CO_2 and H_2O (without drying the recycled gas), which emit and absorb over a wide range bands, could change the heat transfer characteristics mainly due to modification of radiation properties. Although the absorption coefficient has changed from 1.88 m^{-1} to 3.95 m^{-1}, the radiation heat flux in the air-case and in the oxy-fuel case are 11643 W/m² and 12006 W/m², respectively.



(a) (b)

Figure 4 – Heat transfer mechanisms within combustion chamber.

6. CONCLUSIONS

Modeling of an available test facility in the literature is carried out using CFD commercial code FLUENT. The mathematical model is based on a Eulerian description for the continuum phase and a stochastic Lagragian description for the coal particles while the combustion process is modeled utilizing the non-premixed method. In the present study, an attempt has been made to compare specially heat transfer characteristics of pulverized coal combustion in air-fired and in oxy-fuel atmospheres. The O_2/CO_2 mixture utilized in this test case has 0.3 as O_2 mole fraction value. The results show similar thermal conditions in both cases with a very small delaying in the flame propagation for the oxy-fuel situation. Although several parameters have been changed in the oxy-fuel case, these preliminary results show a good perspective to obtain approximated conditions inside combustion chambers, specially in those situations related to retrofit power plants. The accuracy of applied models as well as utilized parameters have been investigated by our research group.

7. ACKNOWLEDGEMENTS

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9. NOMENCLATURE

A	Surface area (m^2)
a	Absorption coefficient (m^{-1})
C	Constant value
c	Specific heat (J/kgK)
D	Diffusion rate coefficient
E	Activation energy (J)
f	Mixture fraction and mass fraction
F	Force (N)
g	Gravitational acceleration (m/s^2)
I	Radiation intensity (W/m^2)
k	Turbulent kinetic energy (m^2/s^2)
k	Kinetic rate (s^{-1})
n	Refractive index
R	Gas law constant (8,31x10^3 J/Kmol K)
r	Radial direction
S	Source terms
s	Path length (m)
t	Time (s)
T	Temperature (K)
u	Axial velocity (m/s)
v	Radial velocity (m/s)
x	Axial direction (m)

Greek symbols

Γ	Effective diffusion coeficient
ε	Energy dissipation rate (m^2/s^3) and emissivity
ρ	Density (kg/m^3)
σ	Stefan-Boltzmann constant (5,67x10^{-8} W/m^{2}K)
Φ	Phase function
ϕ	Generic variable
Ω'	Solid angle

Other symbols

$\Re$	Reaction rate

Subscripts

0	Initial
D	Drag
P	Particle
R	Radiation
v	Volatiles
w	Evaporating/boiling material
ϕ	Generic variable
∞	Local of the continuous phase
ox	Oxidant

10. RESPONSIBILITY NOTICE

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