Mathematical modelling of pulverized coal furnaces

Resumen

The aim of this paper is to set and numerically solve a system of equations that models the processes that occur into a pulverized coal furnace. A simple combustion model consisting of six chemical reactions including vaporization and volatilization is introduced. We use Eulerian coordinates for the gas phase and Lagrangian ones for the solid phase. Low Mach number techniques are used to solve the equations for the gas-phase flow. We consider compressible Navier-Stokes equations with the Smagorinsky's model for turbulence. We consider convection, diffusion and radiation heat transfer phenomena. Radiation heat transfer is taken into account by solving the total radiation intensity equation by a six-flux method. Finite element methods are employed to solve the equations of the stablished model. We incorporate the characteristics method to solve the nonlinearity coming from the convective terms. An iterative algorithm to solve the highly coupled problem is proposed. Numerical results for aerodynamics, radiation and combustion of a coal particle obtained for some industrial furnaces are shown.

1 Introduction

The limitations of the energy resources and, on the other hand, the pollutant emission regulations have led to the need of optimizing the design of combustion equipment. Together with these limitations all combustors should satisfy the following requirements: high combustion efficiency, uniformity of outlet gas temperature maximizing the life of the chamber, low pressure loss, reliable and smooth ignition, durability and minimum cost.

The improvement of the performance and the need to satisfy all the listed requirements have promoted the mathematical modelling with subsequent simulation to increase the knowledge about the combustion phenomena because they are easily, quickly and economically adaptable to different geometric configurations and load conditions.

Several studies about the simulation of behavior models in pulverized coal boilers can be seen in [27], [2], [1], [26] and [34].

In this report a mathematical model for the numerical simulation of the pulverized coal combustion in the boiler of a power plant is described and solved.

First the general structure of the process is analyzed. Then the model equations are detailed: those of the *solid phase*, including a combustion model for the coal particles developed by us (see [6] and [5]) and the *gas phase* ones.

The equations are grouped in submodels corresponding to the different physicochemical phenomena involved in the process. For each of them the methods employed for numerical solution are exposed in a summarized way.

The *solid phase* model is a system of ordinary differential equations which is solved by using an one step finite difference method (implicit Euler). Furthermore numerical non-linear equations appear that are solved by using Newton's method.

The resolution of the *gas phase* equations is much more difficult because of its complexity. The momentum equation is a non-linear system of partial differential equations. We consider a *mixed* variational formulation in velocity/pressure, which is solved by using a tetrahedral finite element method of the P_1-bubble type for the velocity components and P_1 for the pressure. To deal with the non-linearity appearing in the convective term a discretization by *characteristics* is used. Because of the properties of the problem we are led to a system where the three components of the velocity are not coupled. It is solved through a conjugated gradient method, preconditioned with the Cahouet matrix (see [10] and [13]).

Another difficulty arises when solving the energy conservation equation due to the importance of the thermal radiation in the heat transfer phenomena. This makes necessary to include the equation of the energy transport by radiation in the model. The resolution of the energy equation is accomplished by using a tetrahedral P_1 finite element method, combined with characteristics for the treatment of the convective term. For solving the radiation intensity equation a six-flux method is used for the discretization of the direction variable, while for spatial variables a finite difference method having the particularity of reducing the three-dimensional problem to a collection of monodimensional ones is introduced.

For the numerical computation of the mass fractions of the chemical species we solve the conservation equations by using a piecewise linear finite element method with a tetrahedral mesh. The characteristics method is also used for the treatment of the convective term.

In the last part of the report reference is made to the algorithm for the whole model, that it has been implemented in a computer through a FORTRAN program. Finally, graphic output is included with the results obtained for data supplied by the Electric Power Plant of ENDESA (As Pontes).

The analysis of the results given by numerical simulation permits to know the behavior of the boiler and to judge whether they are satisfactory or, on the contrary, it presents aspects to be improved. Then successive executions of the simulation program, incorporating changes in the operating conditions or in the boiler design, would make possible the correction of the detected defects and, in fact, the optimization of the process.

2 The combustion process

2.1 General description

First we describe the combustion process beginning by the geometric domain where it takes place.

The structure of a furnace of the Electric Power Plant of ENDESA (As Pontes) can be seen in the figure 1.

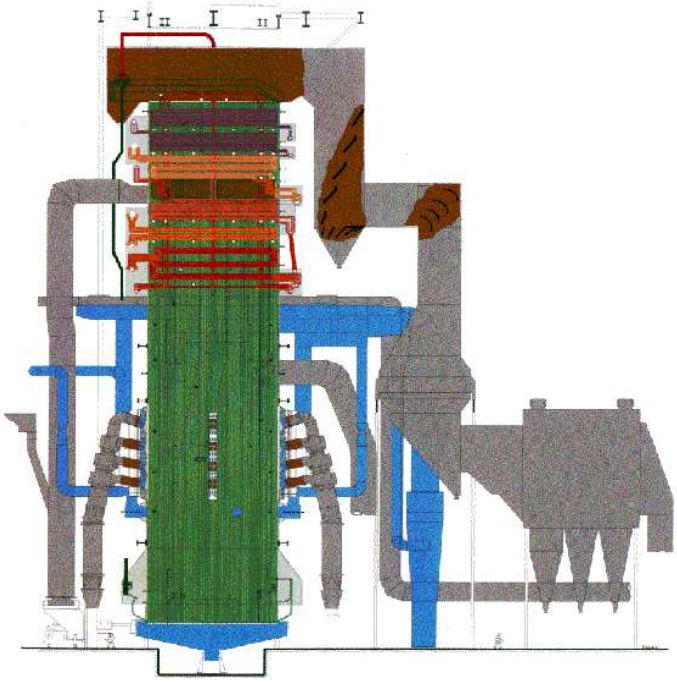


Figura 1: Scheme of the furnace

At given levels inlets exist through which recycled gases are introduced and they drag the pulverized coal, together with fresh air.

Also, some openings exist for the rising of the recirculating gases to the "resuction ducts", which can be in the zone of the fireplace or higher up. Figure 1 shows a furnace where the resuction ducts are out of the fireplace in the zone called "convective". As our interest is centered in the zone where burners are located, we will delimit the geometric domain through an imaginary horizontal plane, across which gases leave the fireplace on the way to the convective zone.

The present model only pretends to study what happens in the fireplace. Furthermore we will suppose that the zone of the fireplace is a spatial area in parallelopiped

form.

As it was previously said, pulverized coal goes into the boiler mixed with recirculating gases at a temperature of 300^oC approximately. Preheated fresh air is also introduced.

In a first stage evaporation of coal moisture and release of volatiles (pyrolysis) takes place. The latter will be burnt in the gas phase. Then combustion of free carbon in the residual char will take place, through a complex chemical process that occurs, first in the surface of the particle and, then, in the gas close to it.

Finally ash remains which, either is deposited in the bottom (and it is taken out through the grid), or leaves the fireplace with the combustion gases and is filtered before the exit of these by the chimney, toward the atmosphere.

The important flows of recirculating gases and fresh air determine speeds larger than 10 m/s. As coal particles are dragged by the gas in their motion, it is understood that aerodynamics is going to determine the flame position; therefore a good knowledge of it becomes fundamental, if we want to simulate precisely the boiler operation.

To this respect fits to indicate that, given the orders of magnitude of the process, the characteristic Reynolds number can be larger than 10^7, something which states that flow is turbulent; this adds greater difficulties to modelling. On the other hand, the temperature variation that gases undergo in the boiler determines important changes in their density, so that the flow is compressible. As it is known, turbulence and compressibility lead to complex models and, consequently, to great computational problems.

On the other hand, the existence of two phases causes the model is composed of two differentiated submodels, though *coupled* between them. The first one describes, in Eulerian coordinates, the mass, momentum and energy conservation of the gases. The second one, that will be expressed in Lagrangian coordinates, translates the conservation laws for coal particles and contains, in particular, the combustion model.

The coupling of both submodels is produced by the following reasons:

- flow of the gas phase determines the position of the particles and the surrounding conditions for the combustion (density, temperature, oxygen and carbon dioxide concentrations, etc.).

- particles act as sources of mass, momentum and energy for the gas phase.

Finally we mention an other important difficulty, which is the fact that heat transfer to the water walls is due, to a great extent, to thermal radiation. This fact forces to introduce the equation of thermal radiation intensity in the model, with the purpose of calculating the corresponding fluxes that appear in the energy equations, both in the gaseous phase and in the coal particles.

2.2 Involved phenomena and main difficulties

Summarizing, the phenomena that characterize the combustion process of the pulverized coal in the fireplace of the boiler of a power plant are the following:

1. Entry of coal particles mixed with recirculating gases and fresh air.
2. Motion of coal particles dragged by gas phase.
3. Moisture evaporation of coal particles.
4. Partial volatilization of coal particles.
5. Combustion of volatilizated gases.
6. Combustion of residual coal (char).
7. Heat transportation by radiation to the water wall.
8. Heat transportation by convection to the higher part of the boiler.

From the analysis of these phenomena we immediately deduce that the fundamental difficulties when modelling the process are the following:

1. Presence of two phases: solid (coal particles) and gaseous.
2. Complex aerodynamics (compressible and turbulent flows).
3. Heat transportation by radiation.
4. Combustion of coal particles (heterogeneous).
5. Coupling of phenomena.

2.3 Mathematical model

A mathematical model, based on the laws of physics, should include the following equations:

- Solid phase
  - *motion*
    - dynamics of a particle
  - *combustion*
    - mass conservation of the components
    - energy conservation
    - kinetics of the chemical reactions

GAS PHASE
- *aerodynamic*
  - mass conservation
  - momentum conservation
  - energy conservation
  - thermal radiation
  - state equation
- *combustion*
  - mass conservation of the species

As we will see below, the corresponding equations to the solid phase are *ordinary differential equations*, while the ones for the gas phase are *partial differential equations*, since the values of the physical magnitudes depend on the position. However they will be time independent since we consider the boiler in stationary state. To proceed to their integration it is necessary to supply *boundary conditions*, that express entry and exit of mass, momentum and energy. These boundary conditions will be calculated through preprocessing programs, from the operating parameters of the boiler supplied by the manager.

By solving these equations at each point of the boiler the values of the physical magnitudes that define the process will be obtained. More precisely:

SOLID PHASE

motion	position and velocity of the particles
kinetic	mass of each species in the particle, sources of mass to the gas phase
energy	temperature of the coal particles, sources of energy to the gas phase

GAS PHASE

cons. momentum	velocity, pressure
cons. mass	divergence of the velocity
cons. energy	temperature, heat to water walls
thermal radiation	radiation flux to water walls
cons. of species	mass fractions
state equation	density

3 Solid phase

In this section we introduce the equations corresponding to the solid phase, that is, to coal particles. It is a *Lagrangian* model, so it establishes what occurs to each particle in its motion through the boiler, instead of what happens in a point, anyone but fixed, of it.

First we have the motion equations. Particles are dragged by the gas, and the gravitational force acts on them.

When they arrive to the interior of the boiler and receive heat by conduction and radiation, particles are heated and then a process consisting of evaporation of their moisture, release of volatiles and oxidation of the resulting char starts. This produces increasing of their temperature and decreasing of mass until they are reduced to inert ash.

We have developed a mathematical model to simulate this combustion process, that improves and completes some other existing in the bibliography on the topic (see [17], [16], [19] or [24]). As usually, it is a simplified model that considers global chemical reactions; however we think that it is adequate, in view of the type of process to be modelled and because of the lack of data to consider more complex combustion mechanisms. In any case, the methodology employed for getting the equations is very general and it could be adapted without great difficulties to include other reactions.

3.1 Model of pyrolysis/combustion

This model is composed of heterogeneous reactions that take place in the solid-gas interphase, and homogeneous reactions in the gas phase including combustion of the volatiles and of the carbon monoxide produced by the oxidation of the char. We will suppose that combustion reaction of the volatiles is equivalent to the global combustion reaction of a single molecule $V = C_a H_b O_c S_d$.

1. *Heterogeneous reactions (at the solid-gas interphase)*

   - moisture evaporation:

   $$H_2O_{(s)} \rightarrow H_2O_{(g)} \qquad + (q_5) \tag{1}$$

   - volatilization:

   $$coal \rightarrow V_{(g)} \qquad + (q_4) \tag{2}$$

   - char oxidation (gasification):
     - carbon oxidation by the carbon dioxide on the particle surface with production of carbon monoxide:

     $$CO_2 + C \rightarrow 2\ CO \qquad + (q_1) \tag{3}$$

– carbon oxidation by the oxygen:

$$\frac{1}{2}O_2 + C \rightarrow CO \qquad + (q_2) \tag{4}$$

2. *Homogeneous reactions*

- combustion of volatiles:

$$C_aH_bO_cS_d + \alpha\ O_2 \rightarrow \beta\ CO_2 + \gamma\ H_2O + \zeta SO_2 \qquad + (q_6) \tag{5}$$

($\alpha = \frac{2a+b/2+2c-d}{2}$, $\beta = a$, $\gamma = \frac{b}{2}$ y $\zeta = d$)

- combustion of carbon monoxide:

$$CO + \frac{1}{2}\ O_2 \rightarrow CO_2 \qquad + (q_3) \tag{6}$$

As it was previously said, this combustion model forms a part of a Lagrangian model that follows the evolution of each particle in the interior of the boiler.

Corresponding equations are exposed below. More details, especially about the derivation of the equations, can be seen in references [6] and [5]. For the validity of those equations the hypothesis that Lewis number of the reactants is unity was considered, though this is only necessary to obtain the temperature equation.

A model corresponding to consider solely the combustion reactions of the carbon, that is, those described in (3), (4) and (6) is obtained in [6]. First a model when the reaction in gas phase (6) is infinitely fast is obtained. Furthermore two cases are considered according to the flame being contiguous to the particle surface or separated from it. Then it is supposed that such reaction is not produced (reaction in gas phase is frozen).

This model (and the methodology to obtain it is extended in [5] to a most complex situation where the reactions of evaporation (1), volatilization (2) and combustion of released volatiles (5) are also included. It is also supposed that the combustion reaction of volatiles is infinitely fast or frozen.

The meaning of each variable can be seen in the notation table appearing at the end of this report.

3.2 Equation for each particle

Below we show conservation equations of the solid phase. It is customary to assume in modelling of pulverized coal combustion that particles are burnt uniformly on its surface.

The model below extends that obtained by Libby and Blake [17] to a more general kinetic situation including moisture evaporation and volatilization. The same methodology that Liñán [18] is used, that is, asymptotic analysis for the limit case

of high activation energy. More references on this topic are [16], [22], [23], [24], [20], [21] or [19].

Furthermore, we consider that particle with radius δ_s (see figure 2) is porous, that is, it does not reduce its size when is burnt but makes it through pores.

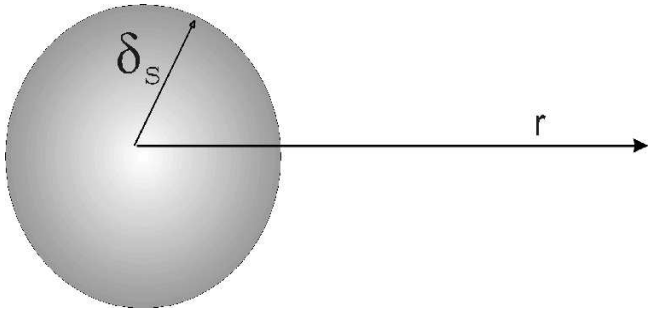


Figura 2: Coal particle

Because reactions in gas phase are supposed to be infinitely fast a "diffusion flame" is produced (i.e., it is determined by the oxygen arrival by diffusion from the surrounding gas) at a distance r_f of the center of the particle. In the case of separated flame sheet ($r_f > \delta_s$) we have a situation as in the figure 3.

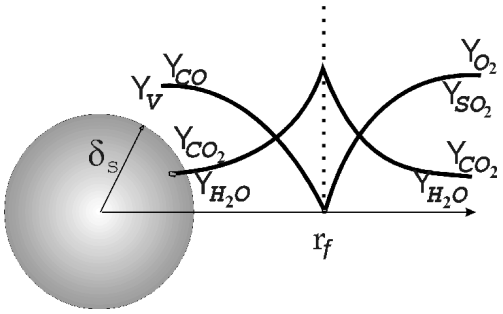


Figura 3: *Separated diffusion flame*

1. *Motion equation*

   In the study of the motion of the pulverized coal particles only gravity and aerodynamic drag forces are meaningful (see [32] or [33]). Then under the hypothesis of particles have spherical form and they are not fragmented during combustion, the following equations result for the motion (see [32]):

$$m_s \frac{dv_s}{dt} = m_s \frac{3}{16} \frac{\mu_g}{\rho_s \delta_s^2} C_D Re(v - v_s) + m_s g \tag{7}$$

$$\frac{dx_s}{dt} = v_s \tag{8}$$

where Re, the Reynolds number based in the relative velocity of the particle as constrasted with the gas one, and C_D are given by

$$Re = \rho_g \mid v - v_s \mid \frac{2\delta_s}{\mu_g}$$

$$C_D = \begin{cases} \dfrac{1 + 0.15Re^{0.687}}{Re/24} & \text{if } Re \leq 1000 \\ 0.44 & \text{other case} \end{cases}$$

with initial conditions:

$$\begin{aligned} v_s(0) &= v_{s0} \\ x_s(0) &= x_{s0} \end{aligned}$$

2. *Equations for the mass of the particle constituents*

By matter balance, the mass of each constituent of the particle can be related to the reaction rates, where these are defined as the mass of substance that reacts per unit volume and time. Furthermore it is considered that ash is an inert species, that is, it does not react. Then equations for the mass of the particle constituents are written as (see [32])

$$\frac{d\rho_{H_2O}}{dt} = -B_5 e^{-\frac{E_5}{\mathcal{R}T_s}} \rho_{H_2O} = -\frac{3k}{\delta_s^2 c_p} \lambda_5 \tag{9}$$

$$\frac{d\rho_V}{dt} = -B_4 e^{-\frac{E_4}{\mathcal{R}T_s}} \rho_V = -\frac{3k}{\delta_s^2 c_p} \lambda_4 \tag{10}$$

$$\frac{d\rho_C}{dt} = -\frac{3k}{\delta_s^2 c_p} [\lambda_1 + \lambda_2] \tag{11}$$

$$\rho_s = \rho_{H_2O} + \rho_V + \rho_C + \rho_{ash}$$

where $\lambda_i = \dfrac{\dot{m}_i c_c}{k\delta_s}$ is the notation for i reaction rate, and with initial conditions:

$$\begin{aligned} \rho_{H_2O}(0) &= \rho^0_{H_2O} \\ \rho_V(0) &= \rho^0_V \\ \rho_C(0) &= \rho^0_C \\ \rho_s(0) &= \rho^0_s \end{aligned}$$

3. *Equations for the combustion rates of the char*

By integrating the classic linear combinations of the quasi-stationary conservation equations for the gas phase we obtain the equations written below. The fact that Shvab-Zeldovich coupled functions follow the same conservation laws as a passive scalar is used for this. Furthermore, as it was already said, it was assumed that reactions in gas phase are infinitely fast. For more details on the methodology employed in the derivation of these equations see [5].

Though for the validity of equations of the reaction rates it is not necessary, assumption of Lewis number of the reactants equals to one is made because it is necessary to obtain the energy conservation equation given below.

The case $f \leq 1$ or $e^{\lambda} \leq f$, corresponds to the flame contiguous to the particle surface, while the other case corresponds to the flame separated from it.

We have (see [5]):

(a)

$$\lambda_1 = \mathcal{K}_1 F_1(\lambda_1, \lambda_2, \lambda_4, \lambda_5) \tag{12}$$
$$\lambda_2 = \mathcal{K}_2 F_2(\lambda_1, \lambda_2, \lambda_4, \lambda_5) \tag{13}$$

(b)

$$F_1 = \frac{1}{\lambda}\left(Y_{1g}\lambda e^{-\lambda} + \frac{11}{3}[\lambda_1+\lambda_2] + \frac{44\beta}{M_{vol}}\lambda_4 - (\frac{11}{3}[\lambda_1+\lambda_2] + \frac{44\beta}{M_{vol}}\lambda_4)e^{-\lambda}\right)$$
$$F_2 = \frac{1}{\lambda}\left(Y_{2g}\lambda e^{-\lambda} - \frac{8}{3}[\lambda_1+\lambda_2] - \frac{32\alpha}{M_{vol}}\lambda_4 - (-\frac{8}{3}[\lambda_1+\lambda_2] - \frac{32\alpha}{M_{vol}}\lambda_4)e^{-\lambda}\right)$$

if $f \leq 1$ or $e^{\lambda} \leq f$,

$$F_1 = \frac{1}{\lambda}\left(Y_{1g}\lambda e^{-\lambda} + \frac{11}{3}[\lambda_1+\lambda_2] + \frac{44\beta}{M_{vol}}\lambda_4 - (\frac{11}{3}[\lambda_1+\lambda_2] + \frac{44\beta}{M_{vol}}\lambda_4)e^{-\lambda} - (\frac{22}{3}\lambda_1 + \frac{11}{3}\lambda_2 + \frac{44\beta}{M_{vol}}\lambda_4)(1-e^{-\lambda}f)\right)$$
$$F_2 = \frac{1}{\lambda}\left(Y_{2g}\lambda e^{-\lambda} - \frac{8}{3}[\lambda_1+\lambda_2] - \frac{32\alpha}{M_{vol}}\lambda_4 - (-\frac{8}{3}[\lambda_1+\lambda_2] - \frac{32\alpha}{M_{vol}}\lambda_4)e^{-\lambda} - (-\frac{8}{3}\lambda_1 - \frac{4}{3}\lambda_2 - \frac{32\alpha}{M_{vol}}\lambda_4)(1-e^{-\lambda}f)\right)$$

otherwise.

(c)

$$\lambda = \lambda_1 + \lambda_2 + \lambda_4 + \lambda_5$$

(d)

$$f = 1 + \frac{Y_{2g}\lambda}{\frac{8}{3}[\lambda_1 + \lambda_2] + \frac{32\alpha}{M_{vol}}\lambda_4}$$

(e)

$$\mathcal{K}_i = B_i e^{-\frac{E_i}{\mathcal{R}T_s}} \rho_g \frac{T_g}{T_s} \frac{\delta_s c_p}{k}, \quad i = 1, 2$$

4. *Energy conservation of the particle*

Below we write the equation of the energy balance where conduction, convection and radiation are considered as forms of energy transportation. The equation is obtained with the same procedure that equations of conservation of species. For this hypothesis of uniform temperature of the particle, that is spatially constant in all the particle, is made.

$$\begin{aligned} c_s \frac{d(m_s T_s)}{dt} &= 4\pi\delta_s k \left\{ (T_g - T_s)\frac{\lambda}{e^\lambda - 1} + [\frac{q_3}{c_p}(\frac{14}{3}\lambda_1 + \frac{7}{3}\lambda_2) + \frac{q_6}{c_p}\lambda_4] \right\} \\ &+ \frac{4\pi\delta_s k}{c_p} \sum_{\substack{i=1 \\ i\neq 3}}^{5} q_i\lambda_i + 4\pi\delta_s^2\xi \left(\int_{S^2} I dS(\omega) - \sigma T_s^4 \right) + c_s T_s \frac{dm_s}{dt} \end{aligned}$$

if $f \leq 1$ or $e^\lambda \leq f$,

$$\begin{aligned} c_s \frac{d(m_s T_s)}{dt} &= 4\pi\delta_s k \left\{ (T_g - T_s)\frac{\lambda}{e^\lambda - 1} + [\frac{q_3}{c_p}(\frac{14}{3}\lambda_1 + \frac{7}{3}\lambda_2) + \frac{q_6}{c_p}\lambda_4]\frac{f-1}{e^\lambda - 1} \right\} \\ &+ \frac{4\pi\delta_s k}{c_p} \sum_{\substack{i=1 \\ i\neq 3}}^{5} q_i\lambda_i + 4\pi\delta_s^2\xi \left(\int_{S^2} I dS(\omega) - \sigma T_s^4 \right) + c_s T_s \frac{dm_s}{dt} \end{aligned}$$

otherwise.

with the initial condition:

$$T_s(0) = T_{s0}$$

3.3 Computation of sources for the gas phase

When we integrate the motion and the combustion model of coal particles in the fireplace we obtain the sources of mass (total and for each species) and energy (total and radiant) going from the solid phase to the gas phase per unit time.

Pulverized coal contains particles with different sizes moving and burning in a different way. Granulometric analysis provides us the size distribution, i.e. the number of types and, for each type, the mean radius and the percentage in weight.

If we denote N_t the number of types, N_e the number of inlets in the fireplace, Q_j the mass flow of coal introduced through the inlet j ($[kg/s]$) and p_{ij} the percentage of particles of type i in coal, then the expression of the source of mass to the gas per unit volume and time ($[kg/(m^3 s)]$) is given by:

$$f_m(x) = \sum_{j=1}^{N_e} \sum_{i=1}^{N_t} Q_j \frac{p_{ij}}{100} \int_0^{t_{ij}^f} F_m^{ij}(t) \delta(x - x_s^{ij}(t)) dt$$

Analogous expressions to the former, we denote respectively by f_{O_2}, f_{CO_2}, f_{H_2O} and f_{SO_2}, are obtained for the sources of the species O_2, CO_2, H_2O and SO_2.

The corresponding expressions of function F, taking into account the dependence on the particle type (radius) and on the inlet, are (see [5]:

- $$F_m(t) = \frac{4\pi\delta_s k}{c_p}\lambda(t) = \frac{4}{3}\pi\delta_s^3 \frac{d\rho_s}{dt}$$

- $$F_{O_2}(t) = \frac{4\pi\delta_s k}{c_p}\left(-\frac{8}{3}[\lambda_1(t) + \lambda_2(t)] - \frac{32\alpha}{M_{vol}}\lambda_4(t)\right)$$

- $$F_{CO_2}(t) = \frac{4\pi\delta_s k}{c_p}\left(\frac{11}{3}[\lambda_1(t) + \lambda_2(t)] + \frac{44\beta}{M_{vol}}\lambda_4(t)\right)$$

- $$F_{H_2O}(t) = \frac{4\pi\delta_s k}{c_p}\left(\lambda_5(t) + \frac{18\gamma}{M_{vol}}\lambda_4(t)\right)$$

- $$F_{SO_2}(t) = \frac{4\pi\delta_s k}{c_p}\frac{64\zeta}{M_{vol}}\lambda_4(t)$$

Next we write the energy source. Energy that one particle transfers to the ambient gas by conduction and convection, per unit time, is (see [5]):

$$F_e(t) = 4\pi\delta_s k\left\{(T_s - T_g)\frac{\lambda}{e^\lambda - 1} + (1-\gamma)\left[\frac{q_3}{c_p}(\frac{14}{3}\lambda_1 + \frac{7}{3}\lambda_2) + \frac{q_6}{c_p}\lambda_4\right]\right\} - c_s T_s \frac{dm_s}{dt},$$

where

$$\gamma = \begin{cases} 1 & \text{if } f \leq 1 \text{ or } e^{\lambda} \leq f, \\ \dfrac{f-1}{e^{\lambda}-1} & \text{other case.} \end{cases}$$

With regard to the emitted radiant energy we have the expression:

$$F_{re}(t) = 4\pi\delta_s^2 \xi \sigma T_s(t)^4.$$

Finally, the radiant energy absorbed by the particle and transformed into internal energy is

$$F_{ra}(t) = 4\pi\delta_s^2 \xi \int_{S^2} I dS(\omega).$$

3.4 Numerical solution

The model of the solid phase that we have described consists of a set of ordinary differential equations and non-linear equations to determine the combustion rates.

An one step implicit finite difference method has been used for numerical solution. In each step, we have to solve a non-linear equation (for the temperature) and a system (for λ_1 and λ_2). This is done by using the Newton's method. Next we detail these methods and equations where they have been used.

The numerical solution of the mass conservation equations (9) and (10) is made with an one step implicit finite difference method, namely

$$\frac{\rho_A^{n+1} - \rho_A^n}{\Delta t} = -B_i e^{-E_i/\mathcal{R}T_s^n} \rho_A^{n+1} \Rightarrow \rho_A^{n+1} = \rho_A^n \frac{1}{1 + \Delta t B_i e^{-E_i/\mathcal{R}T_s^n}}$$

where A=H_2O or V and i=4 ó 5, respectively. The same equations give us the combustion rates of evaporation and volatilization reactions λ_i, as

$$\lambda_i^{n+1} = -\frac{\rho_A^{n+1} - \rho_A^n}{\Delta t} \frac{\delta_s^2 c_p}{3k}$$

The computation of combustion rates of the char is made by solving the non-linear algebraic system (12) and (13) through the Newton's method, and then we obtain a sequence $\{\lambda^{n+1,k}\}_k$ that converges to the solution of the system λ^{n+1}, namely

$$\lambda^{n+1,k+1} = \lambda^{n+1,k} - (Dg(\lambda^{n+1,k}))^{-1} g(\lambda^{n+1,k})$$

where

$$\lambda = (\lambda_1, \lambda_2)$$
$$g(\lambda) = (\lambda\lambda_1 - \mathcal{K}_1 \lambda F_1(\lambda_1, \lambda_2), \lambda\lambda_2 - \mathcal{K}_2 \lambda F_2(\lambda_1, \lambda_2))$$

and $Dg(\lambda^{n,k})$ is the jacobian matrix of g in $\lambda^{n,k}$.

Once we have the combustion rates of the char we just can solve the carbon density in the particle by using the equation (11), through the one step finite difference method

$$\rho_C^{n+1} = \rho_C^n - \Delta t \, \frac{3k}{\delta_s^2 c_p}(\lambda_1^{n+1} + \lambda_2^{n+1})$$

For the solution of the energy equation for one particle, we use again an one step implicit finite difference method. The difficulty arises from the fact that T_s is the solution of a non-linear equation, because of the fourth-degree term that appears in the thermal radiation; more precisely, we get

$$a(T_s^{n+1})^4 + bT_s^{n+1} = c$$

where a, b and c are expressions, arising from the energy equation and from the discretization of the time derivative. Because of this we use the Newton's method to approximate the solution; we have

$$T_s^{k+1} = \frac{3a(T_s^k)^4 + c}{b + 4a(T_s^k)^3}$$

Finally the ordinary differential equations (7) and (8) are integrated exactly. For this is enough to suppose constant gas velocity over the short period of time of integration of the equation. In this case equation (7), which determines the velocity of the particle, can be integrated formally to give

$$v_s = v - (v - v_{s0})e^{-\Delta t/\tau} + g\tau(1 - e^{-\Delta t/\tau})$$

where τ is the characteristic time defined by

$$\tau = \frac{\rho_s \delta_s^2}{18\mu_g f}$$

and

$$f = \frac{C_D Re}{24}.$$

4 Gas phase

In this section we describe the different submodels used to simulate the flow of gases in the boiler. They are the related to aerodynamics, energy transfer and mass transfer of the different species.

4.1 Aerodynamic

Aerodynamics constitutes certainly one of the most difficult and important parts of the model.

We recall that, because of the existence of zones with different temperature, important changes in density of the gases are produced, therefore it is necessary to use a compressible model.

On the other hand, high Reynolds number states that flow is turbulent. To take into account this feature, and with the purpose of calculating the effective viscosity, we have used a *turbulence model*; more precisely Smagorinsky's model due to its simplicity and reduced computational cost. The incorporation of other more complex models, as the classic $k-\epsilon$, should be made without greater difficulties.

Finally one may highlight that, because Mach number is low, the approximation of "isobaric" model can be considered, that is, it is possible to suppose that pressure is spatially homogeneous in the state equation. This simplification, usual in this type of combustion problems, allows us to eliminate the acoustics waves and, as we will see, to adapt the numerical techniques developed for numerical computation of incompressible flows.

4.1.1 Equations of the model

1. *Conservation of the mass*

$$\nabla \cdot (\rho \vec{v}) = f_m \tag{1}$$

2. *Conservation of the momentum*

$$\rho \vec{v} \nabla \vec{v} - \nabla \cdot \bar{\bar{\tau}}\,(x,t) + \nabla p = f_m(v_s - \vec{v}) + \rho g \tag{2}$$

where

$$\bar{\bar{\tau}}\,(x,t) = -\frac{2}{3}\mu_e(\nabla \cdot \vec{v})\,\bar{\bar{I}} + \mu_e(\nabla \vec{v} + (\nabla \vec{v})^t)$$

3. *State equation*

$$p = \rho R T \tag{3}$$

where R is the gas constant, given by

$$R = \frac{\mathcal{R}}{M}$$

and M the molecular mass of the mixture, that is,

$$\frac{1}{M} = \sum_{i=1}^{n_{sp}} \frac{Y_i}{M_i}$$

4. *Boundary conditions*

$$\begin{aligned} &\vec{v} = v_e \quad \text{(inlets and grill)}, \\ &\vec{v} = 0 \quad \text{(walls)}. \end{aligned}$$

4.1.2 Turbulence model

We use the Smagorinsky's model (introduced in [31]), where the turbulent viscosity is calculated through the formula:

$$\mu_t = \rho c \hat{h}^2 \mid \nabla\vec{v} + \nabla\vec{v}^t \mid$$

4.2 "Low Mach number" approximation

As already said, because velocities of gases in the boiler are small with respect to the velocity of sound, pressure can be considered, in a first approximation, spatially homogeneous. This means that in the state equation, (but not in the momentum one), pressure can be considered constant and equal to a given fixed value $\bar{p}$ (in the case of the ENDESA power plant at As Pontes this value is slightly lower than the atmospherical pressure).

This simplification allows us to obtain the density, if we know the temperature and the mass fractions, through the formula:

$$\rho = \frac{\bar{p}}{RT} = \frac{constante}{RT}.$$

Once density is calculated we solve the conservation equations of mass and momentum and we obtain the *velocity and pressure fields*. The advantage that provides the "isobaric" character of the flow is that to solve these equations, methods developed for *incompressible* aerodynamics can be used, after some adjustments; it eliminates problems associated with the presence of acoustic waves.

4.2.1 Numerical methods

Once density and divergence of the velocity are known, the solution of the momentum conservation equation has been carried out through a computer program, implementing *finite element methods* and using recent algorithms. This program is of general application and therefore it can be used for flow calculations in other situations. In particular, geometry is completely general.

Although details are provided in references [9] and [7], we collect here, in a reduced way, the main features of the employed methods:

- Time discretization of the convective term $\rho\vec{v}\nabla\vec{v}$ in the equation (2) by the *characteristics method*. More precisely is approximated by

$$\frac{\vec{v}^{n+1}(x) - \vec{v}^{n}(\mathrm{X}^n(x))}{\Delta t}$$

  where $\mathrm{X}^n(x) = \chi^n(x, t^{n+1}; t^n)$, and $\chi^n(x, t; s)$ gives the position at time s of the particle being at position x at time t (see figure 4). χ^n is the solution of the ordinary differential system

$$\begin{cases} \dfrac{d\chi^n(x,t;\tau)}{d\tau} = \vec{v}^n(\chi^n(x,t;\tau)) \\ \chi^n(x,t;t) = x \end{cases}$$

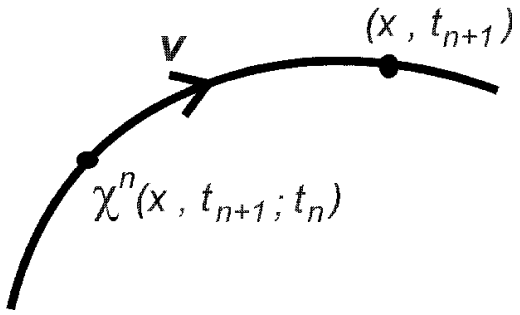


Figura 4: Path or "characteristic"

- Mixed variational formulation in velocity/pressure due to the difficulty of finding finite element spaces that comply with the condition on the divergence of the velocity.

- Spatial discretization through P_1-bubble *finite elements* for the components of the velocity and P_1 for the pressure. It is also called the "mini element" (see [3]).

- Elimination of bubbles by static condensation in the assembly. This is possible because we can express the degrees of freedom of the velocity in barycenters of tetrahedra (bubbles) as linear combinations of the degrees of freedom of the velocity and the pressure in vertices. Therefore the linear system to solve does not involve bubbles, with subsequent simplification in the solution.

- Dual method to solve the discretized problem (pressure as unknown). It results from conversion of the initial linear system, having velocity and pressure as unknowns, to an equivalent system where the unknown is only the pressure.

- Solution of the linear system through a conjugated gradient method, preconditioned with the *Cahouet's matrix* given by (see [10])

$$C_h = \left(\frac{1}{\Delta t} R_h^{-1} + \bar{\mu} I_h^1\right)^{-1}$$

  where $\bar{\mu}$ is an averaged value of the effective viscosity μ_e, and matrices I_h and R_h are discrete approximations of the mass and stiffness terms, respectively.

- Uncoupling of the equations related to the three components of the velocity allowing us to solve three systems with the same matrix.

4.3 Gas phase: heat transfer

Heat transfer in the boiler and toward the water walls is mainly accomplished by convection and radiation.

In order to account for the effect of the convection it is necessary to know the velocity field given by the equation of the gas motion, as well as the density and the specific heat at constant pressure of the mixture which depends on the mass fractions.

On the other hand calculation of radiant heat-flux requires to know the field of the thermal radiation intensity in the fireplace. This leads us to incorporate into the model a new integrodifferential equation, that must be integrated by numerical methods too.

4.3.1 Equations of the model

1. *Energy equation*

   We adopt the following form, valid for Lewis number being unity, the deduction of which can be seen in Kuo [15]

$$\nabla \cdot (\rho h \vec{v}) + \nabla \cdot q_r - \nabla \cdot (\rho D \nabla h) = f_e - f_{ra} + f_{re}, \tag{4}$$

where h is the enthalpy of the gaseous mixture per unit mass. This enthalpy is the sum of the enthalpies per unit mass of species in the mixture, namely

$$h = \sum_{i=1}^{n_{sp}} \left(h_{0i} + \int_{T_0}^{T} c_{pi}(\tau) d\tau \right) Y_i. \tag{5}$$

In the previous expression $c_{pi}(T)$ denotes the specific heat at constant pressure for species i, at temperature T. In general, these functions appear in the bibliography as fourth degree polynomial functions of the temperature, that is,

$$c_{pi}(T) = a_{1i} + a_{2i}T + a_{3i}T^2 + a_{3i}T^3 + a_{4i}T^4$$

2. *Equation of the thermal radiation*

The radiation transfer equation in a medium describes the radiation intensity in any position, throughout its path across a medium that absorbs, emits and scatters it. When scattering is important, it is an integrodifferential equation that may be written as (see [30], [12], [25] or [14])

$$\omega \cdot \nabla_x I + a_s I + a_g I + \sigma_s I - \frac{\sigma_s}{4\pi} \int_{S^2} \phi(\omega^*, \omega) I(\omega^*) dS(\omega^*) = a_s I_{bs} + a_g I_{bg} \tag{6}$$

Once the field I was calculated, the radiant heat-flux vector q_r is given by

$$q_r = \int_{S^2} I \omega dS(\omega)$$

and its divergence, appearing in the energy equation, has the expression

$$\nabla \cdot q_r = \int_{S^2} \left\{ (a_g + a_s) I - a_s I_{bs} - a_g I_{bg} \right\} dS(\omega)$$

3. *Boundary conditions*

Diffuse reflection (in walls):

$$I(x, \omega) = I(x) = \frac{1 - \varepsilon_w}{\pi \varepsilon_w} q_r \cdot n + \frac{\sigma T_w^4}{\pi} \qquad \forall\ \omega / \omega \cdot n < 0. \tag{7}$$

Flux to water walls:

$$q_r \cdot n - \rho D \frac{\partial h}{\partial n} = h_w (T_w - T_a). \tag{8}$$

Temperature of air/gases in inlets and grill:

$$T = T_e. \tag{9}$$

Absorption and scattering coefficients, a_s and σ_s, are functions of the position and depend on the density of the coal particles at the considered point.

We indicate a way of calculating them. We begin by the absorption coefficient a_s. First, we recall that the source of radiation absorbed by particles denoted by f_{ra} was given by (see [25], [30])

$$f_{ra}(x) = \sum_{j=1}^{N_e} \sum_{i=1}^{N_t} Q_j \frac{p_{ij}}{100} \int_0^{t_{ij}^f} 4\pi\delta_s^2 \xi \left(\int_{S^2} I dS(\omega) \right) \delta(x - x_s^{ij}(t)) dt.$$

This term must be equal to

$$\int_{S^2} a_s(\omega, x) I(\omega, x) dS(\omega)$$

representing the radiant energy absorbed by particles at point x. Supposing that a_s does not depend on ω we have:

$$a_s(x) = \frac{f_{ra}(x)}{\int_{S^2} I(\omega, x) dS(\omega)},$$

that is,

$$a_s(x) = \sum_{j=1}^{N_e} \sum_{i=1}^{N_t} Q_j \frac{p_{ij}}{100} \int_0^{t_{ij}^f} \pi\delta_s^2 \xi \delta(x - x_s^{ij}(t)) dt.$$

An analogous reasoning leads us to the following expression for the scattering coefficient:

$$\sigma_s(x) = \sum_{j=1}^{N_e} \sum_{i=1}^{N_t} q_j \frac{p_{ij}}{100} \int_0^{t_{ij}^f} \pi\delta_s^2 \psi \delta(x - x_s^{ij}(t)) dt.$$

4.3.2 Numerical methods

1. *Six-flux method for the radiation*

   Solution of the radiation intensity equation is complex. In fact, the unknown I is function, not only of the considerated point, but also of the direction of propagation. Thus a numerical method must deal with two discretizations, one for each variable.

   For the discretization of the direction variable a flux method is used (see [11], [28] or [29]) where a set of characteristic directions are chosen. We have used a six flux method, which leads to a system of three partial differential equations we detail below.

   To solve this system we have developed two computer programs that implement different methods. The first of them, valid for any type of geometry, uses

a discretization in the spatial variables by piecewise linear *finite elements* with a tetrahedral mesh. The second one initially covers the case where the domain of the model is a parallelopiped. Its advantage is the reduced calculation time that it needs, because of the implementation of an algorithm developed by us, reducing the tridimensional problem to a collection of monodimensional problems.

Next we expose in a short way these techniques and methods. More details can be found in [4] and [8].

First we consider the approximation of the radiation intensity in the following six directions of the space:

$\omega_1^+ = (1,0,0),\ \omega_1^- = (-1,0,0),\ \omega_2^+ = (0,1,0),\ \omega_2^- = (0,-1,0),\ \omega_3^+ = (0,0,1),$ $\omega_3^- = (0,0,-1)$.

We denote by I_i^+ (resp. I_i^-) the approximation of $I(\omega_i^+)$ (resp. of $I(\omega_i^-)$) that we are going to introduce. We also introduce the functions:

$$F_i = I_i^+ + I_i^- \ , \quad q_i = I_i^+ - I_i^- \quad (1 \leq i \leq 3).$$

Then we can prove (see [8]) that the equation of the radiation intensity is reduced to

$$-\frac{\partial}{\partial x_i}\left(\beta \frac{\partial F_i}{\partial x_i}\right) + KF_i - 2\sigma_s s \sum_{\substack{j=1 \\ j\neq i}}^{3} F_j = \frac{2a_g \sigma T^4}{\pi} + \frac{2a_s \sigma T_s^4}{\pi} \ , \quad 1 \leq i \leq 3$$

being

$$\begin{aligned} \beta &= [a + \sigma_s(1 - f + b)]^{-1} \\ K &= a + \sigma_s(1 - f - b) = a + 4\sigma_s s \\ a &= a_s + a_g \end{aligned}$$

$$\begin{aligned} f &= \frac{1}{2}\int_0^{\frac{\pi}{2}} \phi(\theta)\cos^2\theta \sin\theta \ d\theta \\ b &= \frac{1}{2}\int_{\frac{\pi}{2}}^{\pi} \phi(\theta)\cos^2\theta \sin\theta \ d\theta \\ s &= \frac{1}{8}\int_0^{\pi} \phi(\theta)\sin^3\theta \ d\theta \end{aligned}$$

Let

$$q_i = -\beta \frac{\partial F_i}{\partial x_i} \quad (1 \leq i \leq 3)$$

and

$$q_r = \frac{\pi}{2}(q_1, q_2, q_3).$$

Then

$$\nabla \cdot q_r = -\frac{\pi}{2}\sum_{i=1}^{3}\frac{\partial}{\partial x_i}\left(\beta\frac{\partial F_i}{\partial x_i}\right) = 3a_g\sigma T^4 + 3a_s\sigma T_s^4 - a\frac{\pi}{2}\sum_{i=1}^{3}F_i \qquad (10)$$

and by replacing in the energy equation we have:

$$\nabla \cdot (\rho h\vec{v}) + 3a_g\sigma T^4 + 3a_s\sigma T_s^4 - a\frac{\pi}{2}\sum_{i=1}^{3}F_i - \nabla \cdot (\rho D\nabla h) = f_e - f_{ra} + f_{re},$$

or, by eliminating in both sides the radiant energy absorbed and emitted by coal particles,

$$\nabla \cdot (\rho h\vec{v}) + 3a_g\sigma T^4 - a_g\frac{\pi}{2}\sum_{i=1}^{3}F_i - \nabla \cdot (\rho D\nabla h) = f_e.$$

The first term in the right-hand side can also be written as

$$\nabla \cdot (\rho h\vec{v}) = h\nabla \cdot (\rho\vec{v}) + \rho\vec{v} \cdot \nabla h$$

and by using the conservation equation of mass (1) becomes

$$\rho\vec{v} \cdot \nabla h + hf_m + 3a_g\sigma T^4 - a_g\frac{\pi}{2}\sum_{i=1}^{3}F_i - \nabla \cdot (\rho D\nabla h) = f_e. \qquad (11)$$

On the other hand, the boundary conditions (7)-(9) lead to

$$\beta\frac{\partial F_i}{\partial x_i}n_i + \epsilon_w F_i = \frac{2\sigma}{\pi}\epsilon_w T_w^4 \qquad \text{(on the walls)} \qquad (12)$$

$$\frac{\epsilon_w\pi}{2}F_i - \rho D\frac{\partial h}{\partial n} = h_w(T_w - T_a) + \epsilon_w\sigma T_w^4 \qquad \text{(on the walls)} \qquad (13)$$

$$T = T_e \qquad \text{(on inlets and grid)} \qquad (14)$$

2. *Spatial discretization and algorithms of resolution*

Next we describe the methods used for discretization and later resolution of the energy equation (11) and of the discrete radiation equation (10) with boundary conditions (12)-(14).

First the characteristics method is used for discretization of the convective term. For the resolution of the energy equation (calculation of enthalpy and then of temperature) a classical piecewise linear finite element of degree one for a tetrahedral mesh of the domain is used.

On the other one the term $3a_g\sigma T^4$ appearing in the energy equation, is treated in a explicit form, in order to avoid the non-linearity.

Finally, because of the coupling between the energy equation and the radiation intensity equation, we propose the iterative algorithm given below.

(a) **characteristic method for the convective term:**

$$(\rho\vec{v}\cdot\nabla h)(x) = \rho(x)\frac{h^{n+1}(x) - h^n(\mathrm{X}^n(x))}{\Delta t}$$

(b) **iterative algorithm:**

i. Solution of the radiation problem

$$-\frac{\partial}{\partial x_i}\left(\beta\frac{\partial F_i^{n+1}}{\partial x_i}\right) + KF_i^{n+1} - 2\sigma_s s\sum_{\substack{j=1\\ j\neq i}}^{3} F_j^n = \frac{2a_g\sigma(T^n)^4}{\pi} + \frac{2a_s\sigma(T_s)^4}{\pi}, \quad 1\leq i\leq 3,$$

$$\beta\frac{\partial F_i^{n+1}}{\partial x_i}n_i + \epsilon_w F_i^{n+1} = \frac{2\sigma}{\pi}\epsilon_w(T_w^n)^4$$

(collection of onedimensional problems)

ii. Calculation of enthalpy and temperature

$$\rho\frac{h^{n+1}(x) - h^n(\mathrm{X}^n(x))}{\Delta t} + f_m h^{n+1} + 3a_g\sigma(T^n)^4$$
$$-a_g\frac{\pi}{2}\sum_{i=1}^{3} F_i^{n+1} - \nabla\cdot(\rho D\nabla h^n) = f_e.$$

$$\frac{\epsilon_w\pi}{2}F_i^{n+1} - \rho D\frac{\partial h^{n+1}}{\partial n} = h_w(T_w^n - T_a) + \epsilon_w\sigma(T_w^n)^4 \quad \text{(in walls)}$$

These equations are solved by using lagrangian piecewise linear finite elements. For that we make the weak formulation:

$$\int_\Omega \rho(\frac{h^{n+1}(x)-h^n(\mathrm{X}^n(x))}{\Delta t})zdx + \int_\Omega f_m h^{n+1} zdx + \int_\Omega 3a_g\sigma(T^n)^4 zdx$$
$$-\int_\Omega a_g\frac{\pi}{2}(\sum_{i=1}^{3} F_i^{n+1})zdx + \int_\Omega \rho D\nabla h^{n+1}\cdot\nabla z dx =$$
$$\int_\Omega f_e z dx + \int_{\Gamma_w} h_w(T_a - T_w^n)zd\Gamma + \int_{\Gamma_w}\epsilon_w(\frac{\pi}{2}F_i - \sigma(T_w^n)^4)zd\Gamma$$

When we solve this problen we obtain the enthalpy field, h^{n+1}, and then we calculate the termperature, T^{n+1}, by solving the non-linear equations (5) by Newton's method.

4.4 Gas phase: species transportation

The combustion model we have adopted suppose that all chemical reactions take place either on the solid-gas interphase or in the gas close to the particle. At the same time we have supposed that the combustion reactions of the volatiles and of the carbon monoxide produced in the oxidation of the char take place instantaneously and, therefore, they are controlled by this oxidation and by oxygen diffusion.

As a consequence of this, in the gas-phase model we have only considered the following species: nitrogen, carbon dioxide, oxygen, sulphur dioxide and water vapour.

In order to determine the mass fractions of these species in the gas mixture we must write the corresponding conservation laws, including in the right-hand side the contributed mass (or consumed) by the combustion of coal particles.

4.4.1 Equations of the model

Species:

$$1 : CO_2 \qquad 2 : O_2 \qquad 3 : H_2O \qquad 4 : SO_2 \qquad 5 : N_2$$

Equations: (see for example Kuo [15])

$$\nabla\cdot(\rho\vec{v}Y_i) - \nabla\cdot(\rho D\nabla Y_i) = f_i, \quad i = 1,2,3,4.$$

or, equivalently, by using the overall continuity equation (1)

$$\rho\vec{v}\cdot\nabla Y_i + Y_i f_m - \nabla\cdot(\rho D\nabla Y_i) = f_i, \quad i = 1,2,3,4. \tag{15}$$

$$Y_5 = 1 - Y_1 - Y_2 - Y_3 - Y_4$$

Boundary conditions:

$$Y_i = Y_{ie}, \quad \text{(inlets and grid)},$$

$$\frac{\partial Y_i}{\partial n} = 0, \quad \text{(walls and outlets)}.$$

4.4.2 Numerical methods

The previous equations have been solved by using the following numerical techniques

1. **characteristics method for the convective term:**

$$(\rho\vec{v}\cdot\nabla Y)(x) = \rho(x)\frac{Y^{n+1}(x) - Y^n(\mathrm{X}^n(x))}{\Delta t}$$

2. **iterative algorithm:**

$$\rho\frac{Y^{n+1}(x) - Y^n(\mathrm{X}^n(x))}{\Delta t} + f_m Y^{n+1} - \nabla\cdot(\rho D\nabla Y^{n+1}) = f$$

These equations are solved by using a piecewise linear finite element method for a tetrahedral mesh to discretize the following weak formulation

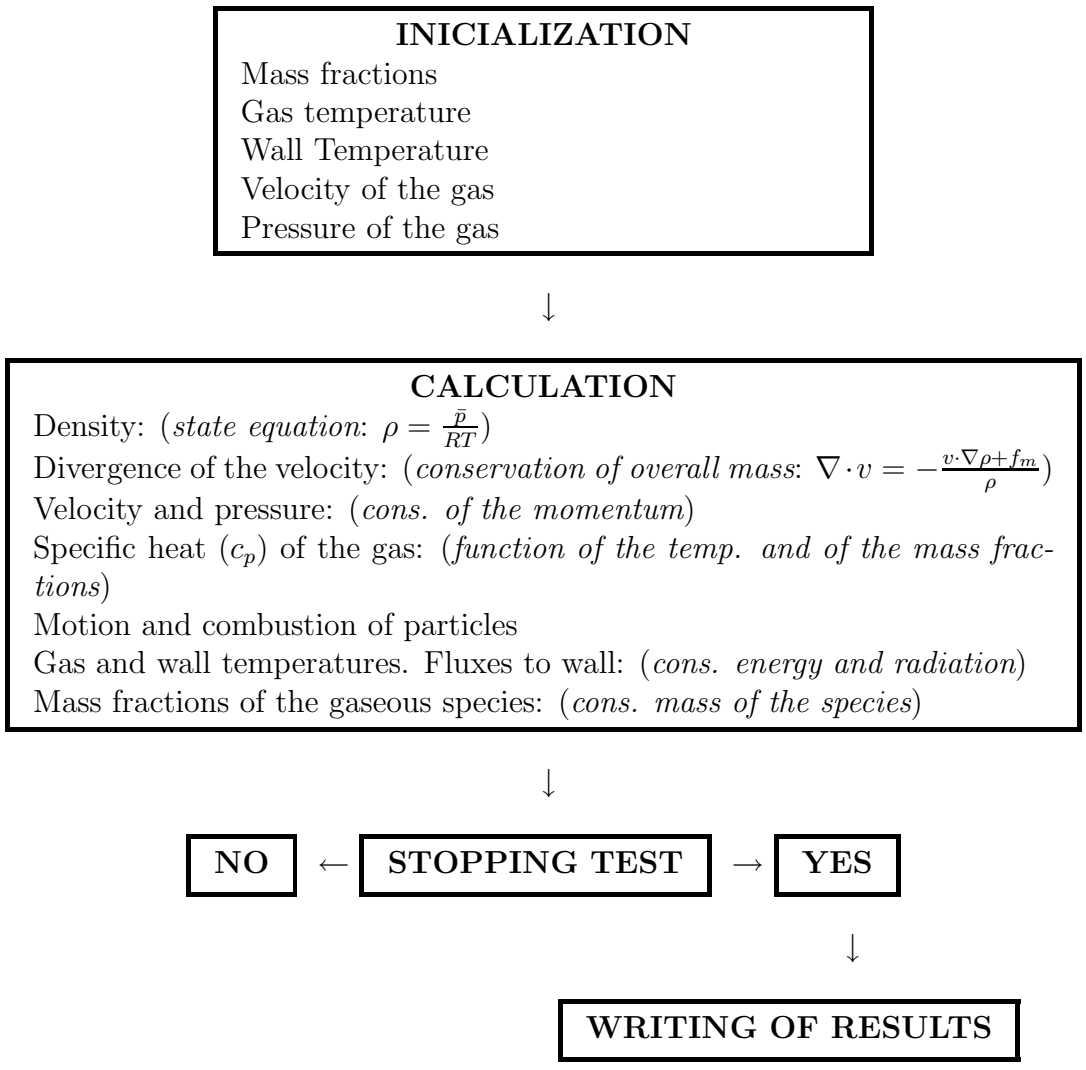
$$\int_\Omega \rho(\frac{Y^{n+1}(x) - Y^n(\mathrm{X}^n(x))}{\Delta t})z dx + \int_\Omega f_m Y^{n+1} z dx$$
$$+ \int_\Omega \rho D\nabla Y^{n+1}\cdot\nabla z dx = \int_\Omega f z dx$$

Note that the finite element matrix depends on the density but not on n. Moreover it is the one appearing in the energy equation. Thus we assembly, block and factorize a single matrix to solve energy and mass fractions equations.

5 Global algorithm

We have just indicated that the different submodels corresponding to the gas-phase and to the solid-phase are coupled. Therefore, if we want to simulate the behaviour of the boiler it is necessary to solve them together.

Next diagram summarizes the iterative algorithm that we have implemented to solve this coupled problem. Furthermore we indicate the equations we solve in each step.



The correspondent program, written in FORTRAN 77, has more than 15.000 lines. We have made a graphical interface with C and X11/Motif in order to make it user-friendly.

6 Numerical results

The results presented below have been obtained with the previous model, for a boiler of the ENDESA Power Plant at As Pontes. The figures 10, 11 and 12 show two side views and a horizontal section of the boiler, where situation of burners can be apreciated. The furnace has six mills, with four levels or "fingers" each one.

Data, both geometrical and operation, have been supplied by ENDESA that has carried out the corresponding measures. Only four mills are operating in the simulation carried out (those marked with letters A, C, D and F in the figure 12). Through the other ones only air is introduced.

Graphical outputs in figures 6, 7, 8 and 9 show some results obtained with the computer program for the model of combustion of particles. More precisely, we show the evolution in time of density, energy source, combustion rate and temperature of one particle moving into the fireplace.

Finally we include graphical outputs with results of the gas phase on two sections -one vertical and an other horizontal, marked with point lines in the figures 10, 11 and 12- the velocity field and, over it, temperatures (figures 13 and 14), pressures (figures 15 and 16) and CO_2 mass fractions (figures 17 and 18).

The finite element mesh used for this simulation has 34.320 tetrahedra and 6762 vertices and it can be seen in the figure 5.

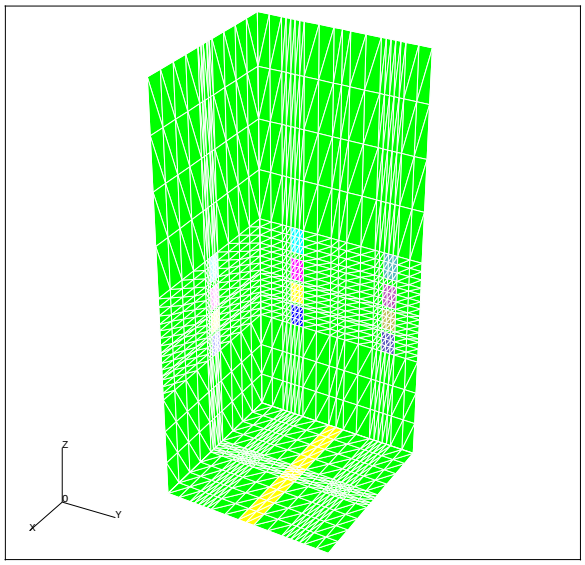


Figura 5: Mesh of the zone of the fireplace of the furnace

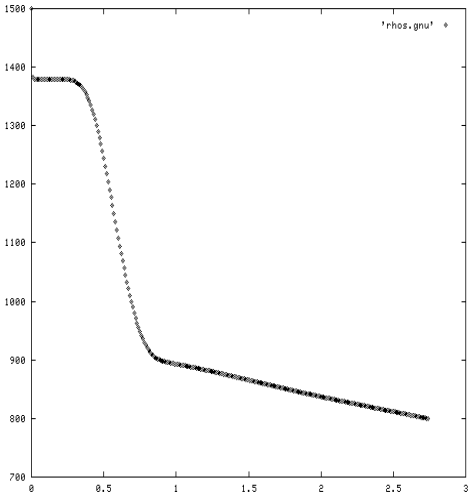


Figura 6: Density (ρ_s)

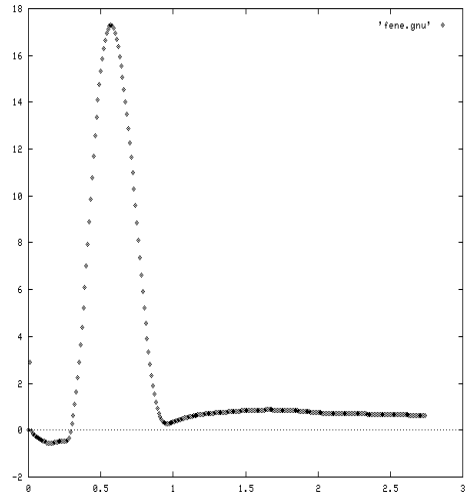


Figura 7: Source of energy (f_e)

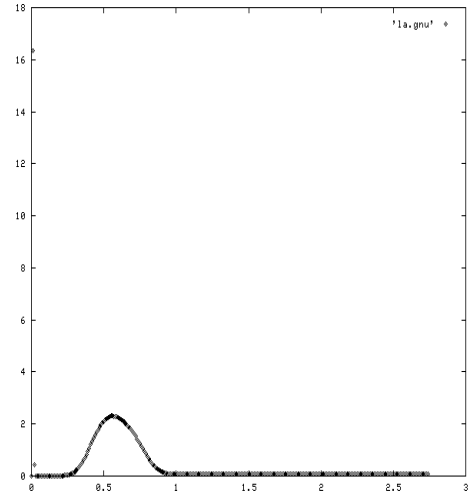


Figura 8: Combustion rate (λ)

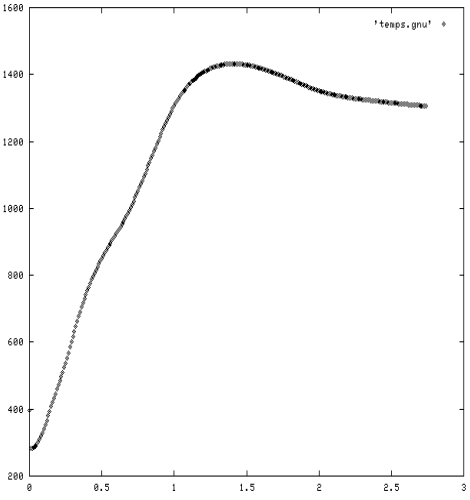


Figura 9: Temperature (T_s)

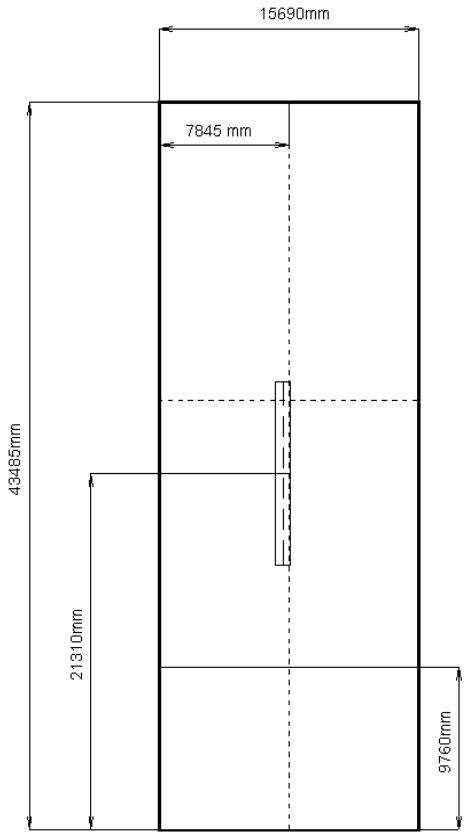


Figura 10: Lateral side view of the boiler

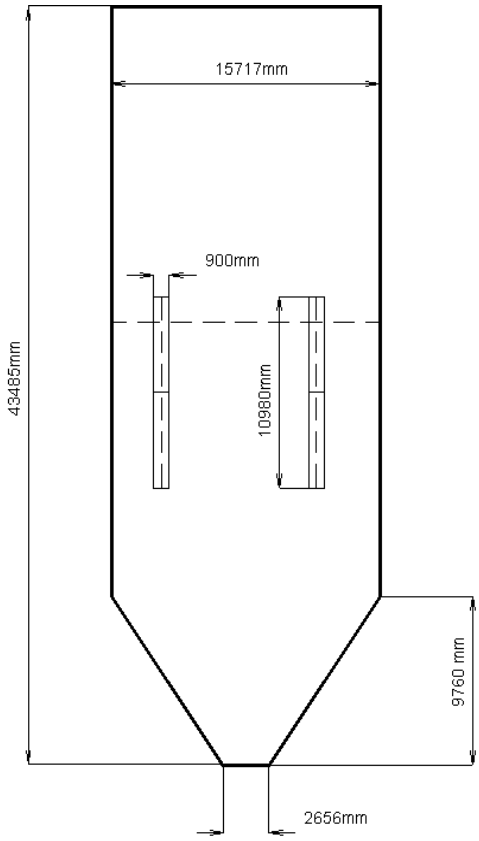


Figura 11: Frontal side view of the boiler

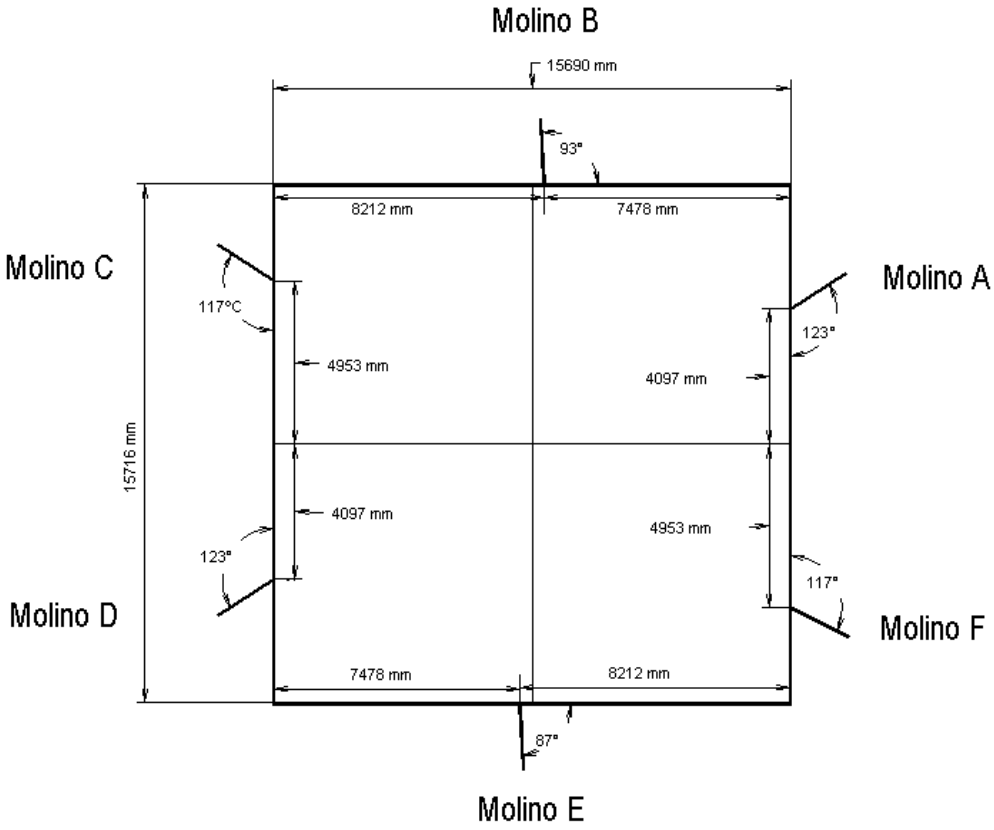


Figura 12: Horizontal section of the boiler

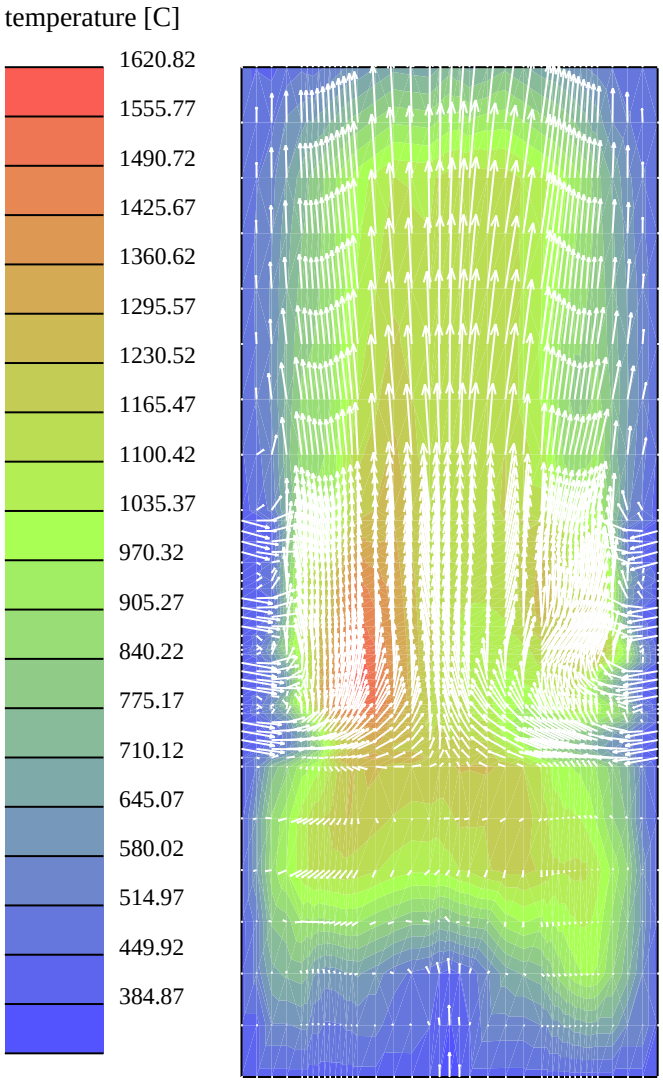


Figura 13: Section $x = 7.845$ with velocity and temperature

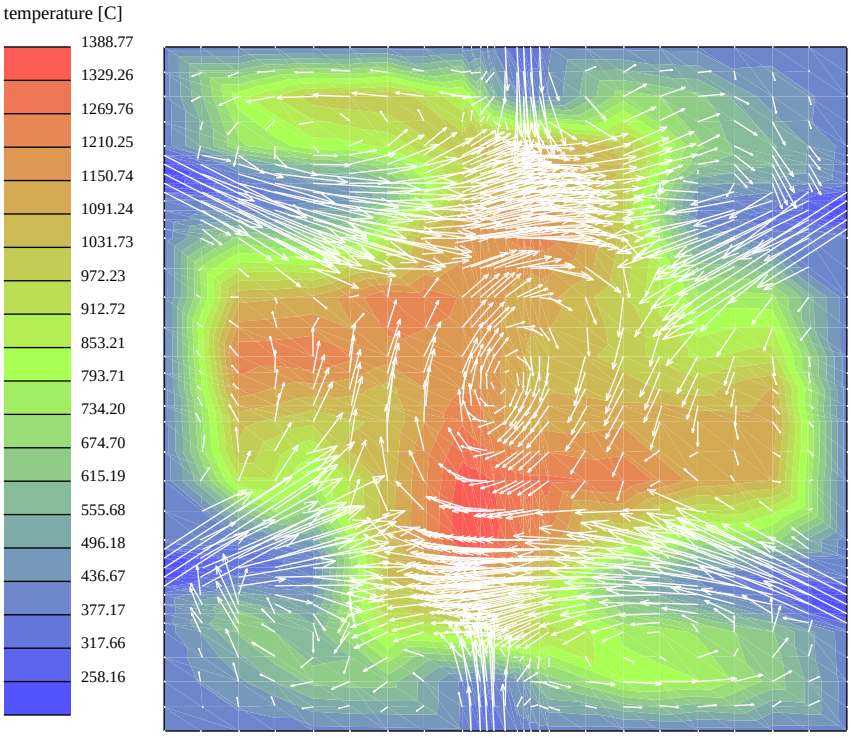


Figura 14: Section $z = 27.8$ with velocity and temperature

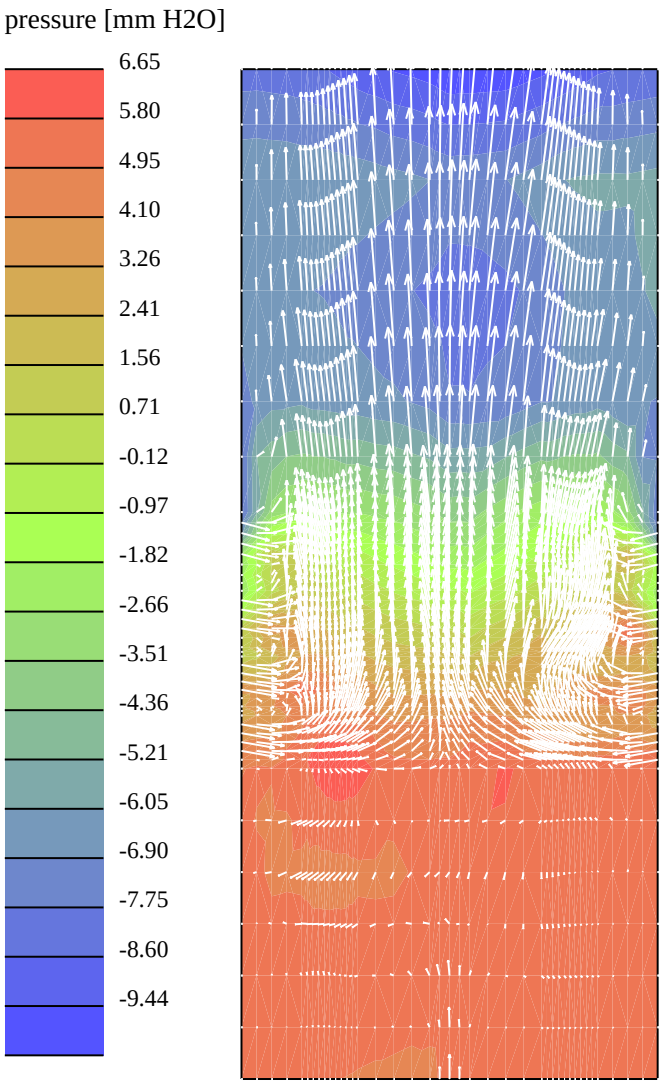


Figura 15: Section $x = 7.845$ with velocity and pressure

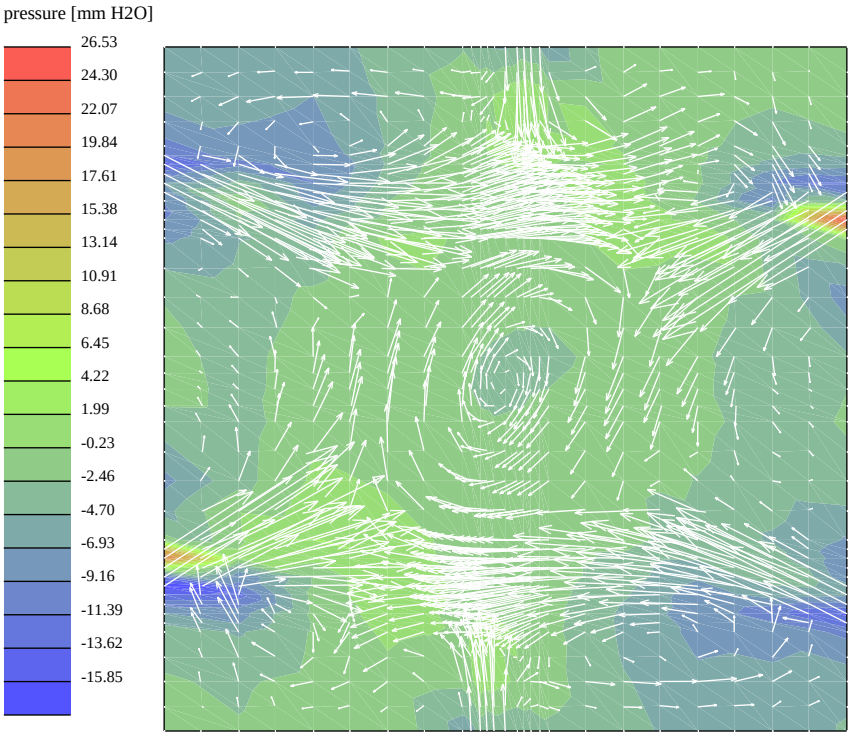


Figura 16: Section $z = 27.8$ with velocity and pressure

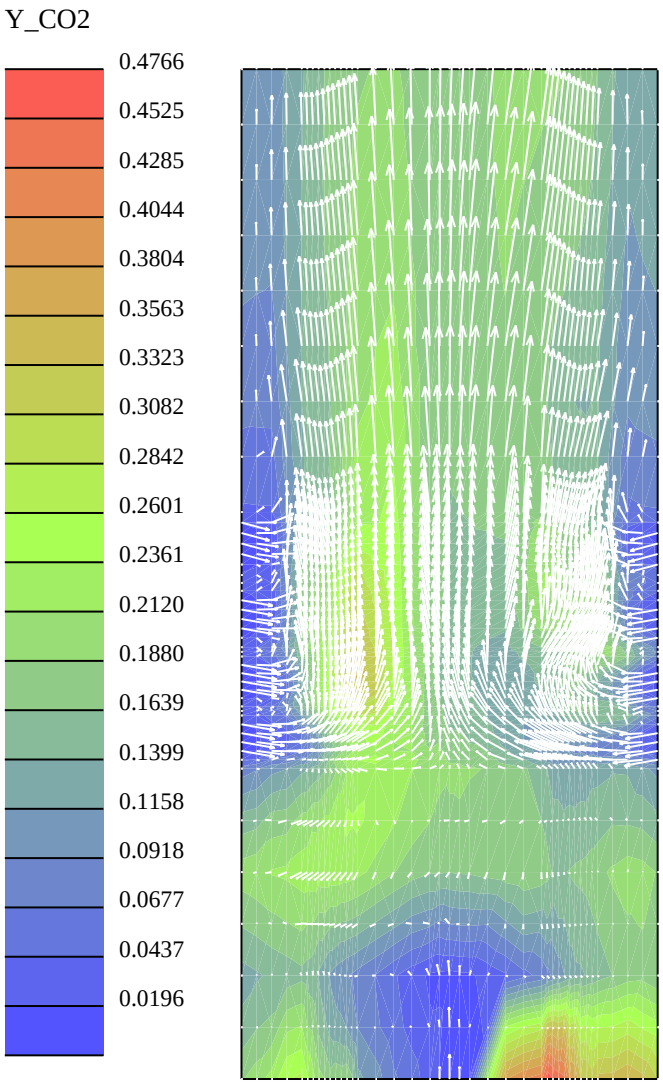


Figura 17: Section $x = 7.845$ with velocity and mass fractions of CO_2

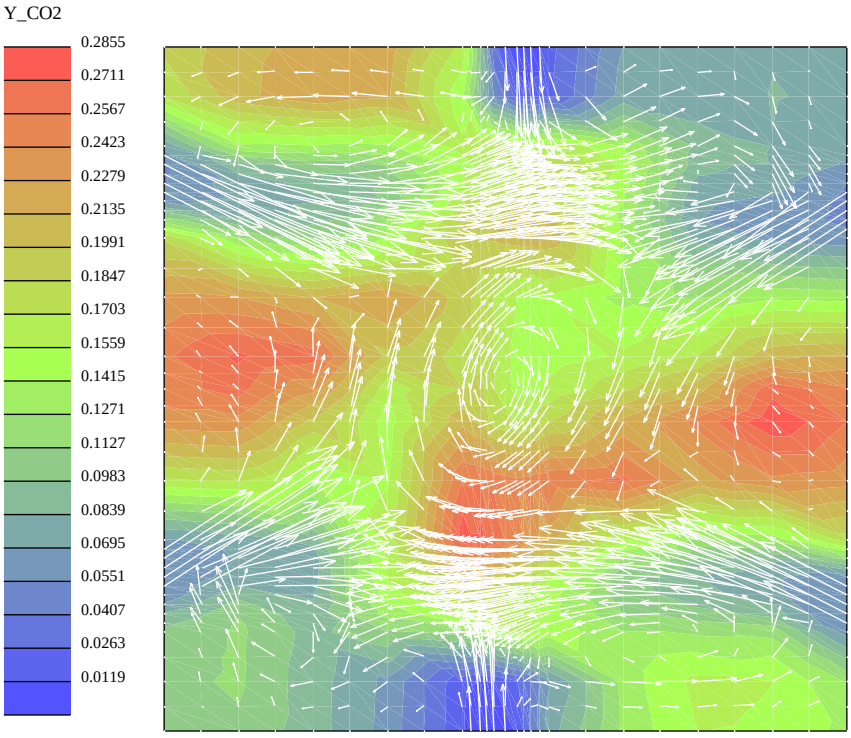


Figura 18: Section $z = 27.8$ with velocity and mass fractions of CO_2

7 Conclusions

We have introduced and numerically solved a mathematical model for the simulation of the combustion process of pulverized coal in a boiler.

It is a tridimensional model that allows us to calculate the thermodynamic variables at each point of the domain. It consists of two parts corresponding to the solid phase (coal particles) and the gas. It is structured in submodels corresponding to the different physical-chemical fenomena involved in the process: motion and combustion of coal particles, aerodynamics, heat transfer/thermal radiation, species transportation. It also includes pre and postprocessing programs to use the libraries MODULEF, GNUPLOT and VIGIE for finite element mesh generation and for visualization of the 2D and 3D results.

These programs have been used to simulate a furnace of the ENDESA Power Plant (As Pontes). Although validation and adjust process are not concluded, the comparison of the first results obtained with the measured values in the Plant can be considered satisfactory. In any case, they can be used to state what are the posibilities of the simulation program we have developed and its potential utility to improve the performance of the combustion process, to explain certain phenomena and to help in the design of new boilers. For example, by changing some of the data and running the program in the computer, it would be possible to see the effect of modifying the flow rate of the recirculating gases.

To conclude, the simulation tool we have developed can be very useful not only to design new boilers, but also to know the behaviour of the existing ones when changes in the type of coal, flow rate of gases/air, orientation of the jets in the burners, etc, are carried out.

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8 Nomenclature list

- a_g: absortion coefficient of the thermal radiation of the gas $[m^{-1}]$
- a_s: absortion coefficient of the thermal radiation of the particles $[m^{-1}]$
- B_i: frecuency factor for reaction i $[m/s]$
- c: adjust parameter (it is taken equal to 0.01)

- C_D: particle aerodynamic drag coefficient
- c_p: specific heat at constant pressure of the gas $[J/(kg\,K)]$
- c_{pi}: specific heat at constant pressure of the species i $[J/(kg\,K)]$
- c_s: specific heat of the particle $[J/(kg\,K)]$
- D: mass diffusion coefficient $[m^2/s]$
- δ_s: radius of the particle $[m]$
- $\delta(x-.)$: Dirac meassure at x
- E_i: activation energy for reaction i $[J/kmol]$
- ϵ_w: adimensional emissivity coefficient of the water walls
- $f_A(x)$: source per unit volume and time of the magnitude A, at x
- $F_A^{ij}(t)$: quantity of the magnitude A per unit time, released at t by a particle of type i introduced in the fireplace by the inlet j
- F_i: radiation fluxes
- ϕ: defraction function
- g: gravitational vector $[9.8\ m/s^2]$
- h: enthalpy per unit mass $[J/kg]$
- $\hat{h}$: characteristic parameter of the mesh size
- h_i: enthalpy per unit mass of the species i $[J/kg]$
- h_{0i}: reference enthalpy per unit mass of the species i $[J/kg]$
- h_w: coefficient of heat transfer to the walls $[W/(m^2K)]$
- I: total intensity of the thermal radiation $[W/(m^2\,str)]$
- $$I_{bs} = \frac{\sigma T_s^4}{\pi}$$
- $$I_{bg} = \frac{\sigma T^4}{\pi}$$

- ψ: adimensional scattering coefficient of the coal particles
- k: thermal conductivity of the gas $[W/(m\,K)]$
- $\lambda_i(t)$: (adimensional) reaction rate i at t
- $m_s(t)$: mass of the particle at t $[kg]$
- M: molecular weight of the mixture $[kg/kmol]$
- M_i: molecular weight of the species i $[kg/kmol]$
- M_{vol}: molecular weight of the volatile combustibles $[kg/kmol]$
- μ_e: effective dynamic viscosity $(\mu_e = \mu_g + \mu_t)$ $[kg/(ms)]$
- μ_g: shear dynamic viscosity of the gas $[kg/(m\,s)]$
- μ_t: turbulent viscosity $[kg/(ms)]$
- $n = (n_1, n_2, n_3)$: exterior unit normal vector to the surface of the boiler
- n_{sp}: number of gaseous species in the gaseous mixture
- p: pressure $[N/m^2]$
- $\bar{p}$: mean pressure in the interior of the fireplace
- p_{ij}: percentage of coal of type i that goes in the fireplace by the inlet j
- q_i: heat of the reaction i $[J/kg]$
- Q_j: mass flow of coal through the inlet j [kg/s]
- q_r: radiant heat-flux vector $[W/m^2]$
- R: gas constant $[J/(K\,kg)]$
- $\mathcal{R}$: universal gas constant $[8.317 \times 10^3\ J/(K\,kmol)]$
- Re: Reynolds number
- ρ: density of the gas $[kg/m^3]$
- $\rho_A(t)$: density of the species A in the particle at t $[kg/m^3]$
- $\rho_g(t) = \rho\,(t, x_s(t))$: density of the gas close to the particle at t $[kg/m^3]$
- ρ_s: density of the particle $[kg/m^3]$

- S^2: unit sphere
- σ: Stefan-Boltzmann constant $[5.6696 \times 10^{-8}\ W/(m^2\, K^4)]$
- σ_s: scattering coefficient of the thermal radiation for the gas because of the presence of coal particles $[m^{-1}]$
- T: temperature of the gas in the fireplace $[K]$
- T_0: reference temperature $[K]$
- T_a temperature of the water in the tubes [K]
- T_e: temperature of the gases in the inlet $[K]$
- $T_g(t) = T\,(t, x_s(t))$: temperature of the gas close to the particle at t $[K]$
- $T_s(t)$: temperature of the particle at t $[K]$
- T_{s0}: initial temperature of the particle $[K]$
- T_w temperature of the water walls [K]
- t_{ij}^f: time that takes the particle to be completely burnt or to leave the fireplace
- $\vec{v}$: velocity of the gas $[m/s]$
- v_e: velocity of the gases in the inlet $[m/s]$
- $v_g(t) = v\,(t, x_s(t))$: velocity of the gas close to the particle at t $[m/s]$
- $v_s(t)$: velocity of the particle at t $[m/s]$
- v_{s0}: initial velocity of the particle $[m/s]$
- ω: unit vector showing directions of radiant transmission
- $x_s(t)$: position of the particle at t $[m]$
- x_{s0}: initial position of the particle $[m]$
- $x_s^{ij}(t)$: position where is the particle at t
- ξ: adimensional coefficient of the thermal radiation emissivity of the particle
- Y_i: mass fraction of the species i [adimensional]
- Y_{ie}: mass fraction of the species i in the inlets [adimensional]
- $Y_{ig}(t) = Y_i\,(t, x_s(t))$: mass fraction of the species i close to the particle at t, being CO_2 the corresponding one to $i = 1$ and O_2 to $i = 2$

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