# Mathematical modelling and numerical solution of group coal combustion

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# Outline

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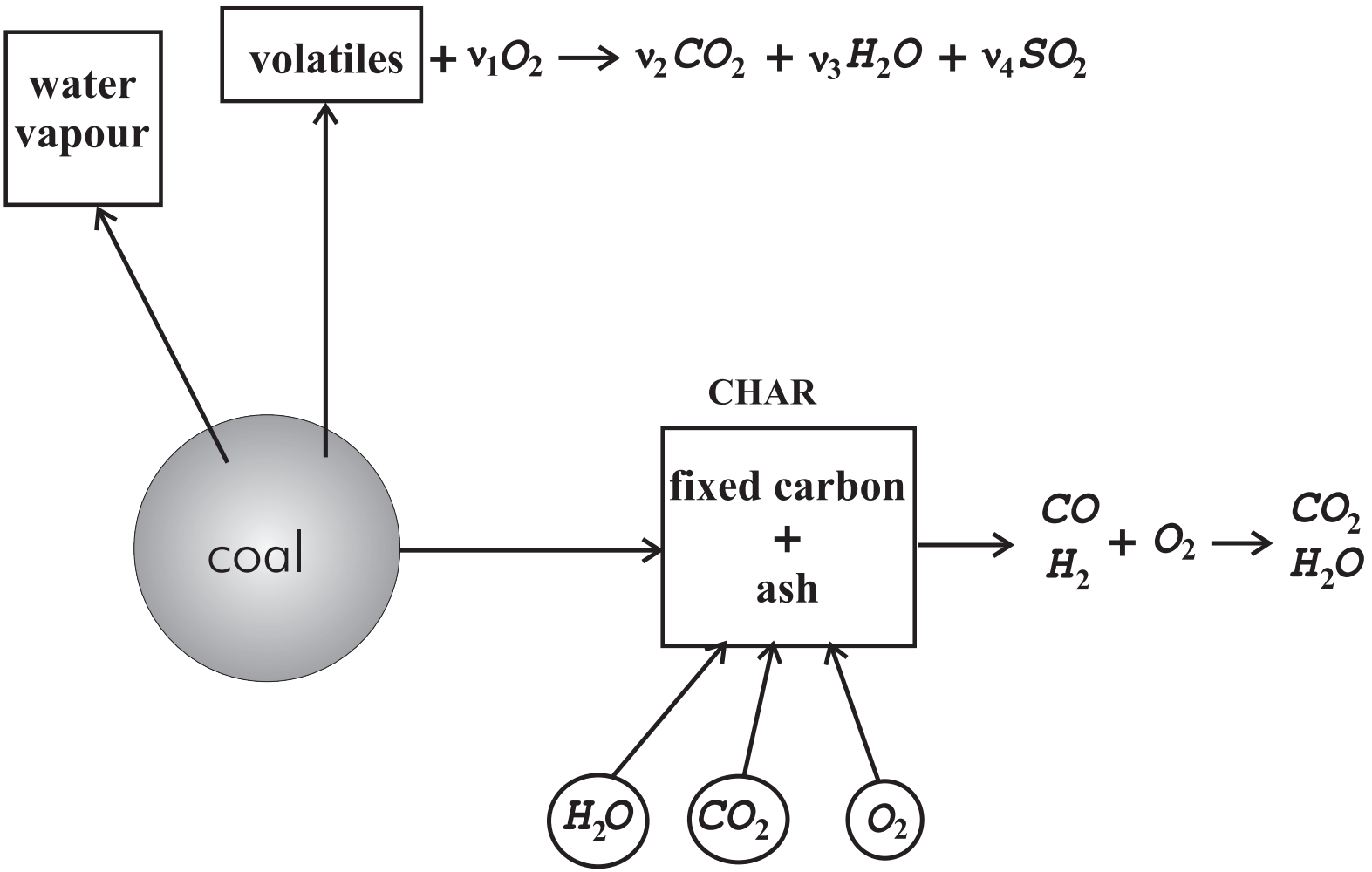
# Coal combustion



# Combustion model

Heterogeneous reactions:

1 $$CO_2 + C_{(s)} \rightarrow 2\ CO \quad + (q_1)$$

2 $$\frac{1}{2}O_2 + C_{(s)} \rightarrow CO \quad + (q_2)$$

3 $$H_2O + C_{(s)} \rightarrow CO + H_2 \quad + (q_3)$$

4 $$V_{(s)} \rightarrow V_{(g)} \quad + (q_4)$$

5 $$H_2O_{(s)} \rightarrow H_2O_{(g)} \quad + (q_5)$$

Gas phase oxidation reactions:

6 $$CO + \frac{1}{2}\ O_2 \rightarrow CO_2 \quad + (q_6)$$

7 $$V_{(g)} + \nu_1\ O_2 \rightarrow \nu_2\ CO_2 + \nu_3\ H_2O + \nu_4\ SO_2 \quad + (q_7)$$

8 $$H_2 + \frac{1}{2}\ O_2 \rightarrow H_2O \quad + (q_8)$$

$q_i$ is the heat released in the $i$-th reaction per unit mass gasified

# Gas phase model

We want to simulate a turbulent mixture of reacting gases where pulverised coal combustion occurs.

In order to obtain a simplified mathematical description of this type of combustion problem, we can assume the following hypotheses:

1. All the diffusion coefficients $\mathcal{D}_i$ of chemical species are equal to $\mathcal{D}$,
2. Lewis number is equal to 1, so

$$k_T = \rho \mathcal{D} c_\pi ,$$

3. Fick's law for the diffusion velocities,
4. Low Mach number. Then, pressure can be assumed to be constant in the state equation.

# Gas phase model

Equations for a turbulent mixture of reacting gases are:

- State equation

$$\overline{\pi} = \rho \mathcal{R} \theta.$$

- Continuity and momentum conservation

$$\frac{\partial \rho_g}{\partial t} + \mathrm{div}(\rho_g \mathbf{v}_g) = f^m,$$

$$\frac{\partial (\rho \mathbf{v}_g)}{\partial t} + \mathrm{div}(\rho \mathbf{v}_g \otimes \mathbf{v}_g) + \mathrm{grad}\pi$$

$$-\mathrm{div}\left( (\mu + \mu_t)(\mathrm{grad}\mathbf{v}_g + \mathrm{grad}\mathbf{v}_g^t) - \frac{2}{3}(\mu + \mu_t)\mathrm{div}\mathbf{v}_g \mathbb{I} - \frac{2}{3}\rho k \mathbb{I} \right) = \rho \mathbf{g}.$$

- Turbulence model: $k - \epsilon$ standard

$$\mu_t = 0.09 \rho \frac{k^2}{\epsilon},$$

$$\frac{\partial (\rho k)}{\partial t} + \mathrm{div}(\rho \mathbf{v}_g k) - \mathrm{div}\left[ (\mu + \mu_t)\, \mathrm{grad} k \right] = P_k - \rho \epsilon,$$

$$\frac{\partial (\rho \epsilon)}{\partial t} + \mathrm{div}(\rho \mathbf{v}_g \epsilon) - \mathrm{div}\left[ \left( \mu + \frac{\mu_t}{1.3} \right) \mathrm{grad} \epsilon \right] = 1.44 \frac{\epsilon}{k} P_k - 1.92 \frac{\epsilon^2}{k}.$$

# Gas phase model

- Mass of each species and energy conservation

$$\mathcal{L}_g(Y^g_{O_2}) = f^m_{O_2} - \frac{4}{7}w_6 - \frac{32\nu_1}{M_{\text{vol}}}w_7 - 8w_8,$$
$$\mathcal{L}_g(Y^g_{CO_2}) = f^m_{CO_2} + \frac{11}{7}w_6 + \frac{44\nu_2}{M_{\text{vol}}}w_7,$$
$$\mathcal{L}_g(Y^g_{H_2O}) = f^m_{H_2O} + \frac{18\nu_3}{M_{\text{vol}}}w_7 + 9w_8,$$
$$\mathcal{L}_g(Y^g_{SO_2}) = f^m_{SO_2} + \frac{64\nu_4}{M_{\text{vol}}}w_7,$$
$$\mathcal{L}_g(Y^g_{CO}) = f^m_{CO} - w_6,$$
$$\mathcal{L}_g(Y^g_{V}) = f^m_{V} - w_7,$$
$$\mathcal{L}_g(Y^g_{H_2}) = f^m_{H_2} - w_8,$$
$$\mathcal{L}_g(h^g_T) = f^e + q_6w_6 + q_7w_7 + q_8w_8 - \text{div}\mathbf{q}_{rg},$$

$w_i$ the rate of the $i$-th reaction

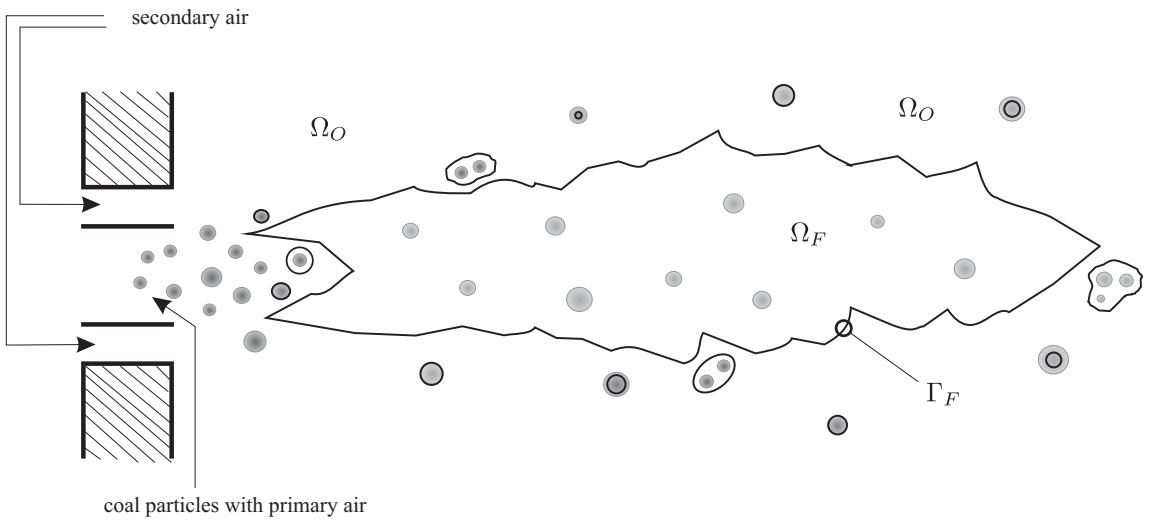
with

$$\mathcal{L}_g(u) = \frac{\partial(\rho_g u)}{\partial t} + \text{div}(\rho_g u\mathbf{v}) - \text{div}(\rho_g \mathcal{D}\text{grad}u).$$

# Gas phase model

## Burke-Schumann hypothesis

Gas phase reactions are frozen or they occur with infinitely fast velocity in a gaseous thin diffusion flame.




Diffusion flame

- $\Omega_0$: Region with oxygen and no fuel
- $\Omega_F$: Region with fuel and no oxygen
- $\Gamma_F$: Diffusion flame

# Gas phase model

In order to obtain equations without the gas phase reaction terms we consider linear combinations of Shvab-Zeldovich type:

## Shvab-Zeldovich scalars

$$
\begin{aligned}
X_1^g &= Y_{O_2}^g - \frac{4}{7}Y_{CO}^g - \frac{32\nu_1}{M_{\text{vol}}}Y_V^g - 8Y_{H_2}^g \\
X_2^g &= Y_{CO_2}^g + \frac{11}{7}Y_{CO}^g + \frac{44\nu_2}{M_{\text{vol}}}Y_V^g \\
X_3^g &= Y_{H_2O}^g + \frac{18\nu_3}{M_{\text{vol}}}Y_V^g + 9Y_{H_2}^g \\
X_4^g &= Y_{SO_2}^g + \frac{64\nu_4}{M_{\text{vol}}}Y_V^g \\
H^g &= h_T^g + q_6 Y_{CO}^g + q_7 Y_V^g + q_8 Y_{H_2}^g
\end{aligned}
$$

## Conservation equations

$$
\begin{aligned}
\mathcal{L}_g(X_1^g) &= f_{O_2}^m - \frac{4}{7}f_{CO}^m - \frac{32\nu_1}{M_{\text{vol}}}f_V^m - 8f_{H_2}^m \\
\mathcal{L}_g(X_2^g) &= f_{CO_2}^m + \frac{11}{7}f_{CO}^m + \frac{44\nu_2}{M_{\text{vol}}}f_V^m \\
\mathcal{L}_g(X_3^g) &= f_{H_2O}^m + \frac{18\nu_3}{M_{\text{vol}}}f_V^m + 9f_{H_2}^m \\
\mathcal{L}_g(X_4^g) &= f_{SO_2}^m + \frac{64\nu_4}{M_{\text{vol}}}f_V^m \\
\mathcal{L}_g(H^g) &= f^e + q_6 f_{CO}^m + q_7 f_V^m + q_8 f_{H_2}^m - \nabla\cdot\mathbf{q}_{rg}
\end{aligned}
$$

# Gas phase model

$$X_1^g = Y_{O_2}^g - \frac{4}{7} Y_{CO}^g - \frac{32\nu_1}{M_{\text{vol}}} Y_V^g - 8 Y_{H_2}^g$$

determines the region in which we are:

1. If $X_1^g > 0 \Rightarrow$ Domain $\Omega_O \Rightarrow Y_{CO}^g = Y_V^g = Y_{H_2}^g = 0$

$$\begin{aligned} Y_{O_2}^g &= X_1^g \\ Y_{CO_2}^g &= X_2^g \\ Y_{H_2O}^g &= X_3^g \\ Y_{SO_2}^g &= X_4^g \\ h_T^g &= H^g \end{aligned}$$

# Gas phase model

$$X_1^g = Y_{O_2}^g - \frac{4}{7} Y_{CO}^g - \frac{32\nu_1}{M_{\text{vol}}} Y_V^g - 8 Y_{H_2}^g$$

determines the region in which we are:

1. If $X_1^g > 0 \Rightarrow$ Domain $\Omega_O \Rightarrow Y_{CO}^g = Y_V^g = Y_{H_2}^g = 0$
2. If $X_1^g < 0 \Rightarrow$ Domain $\Omega_F \Rightarrow Y_{O_2}^g = 0 \Rightarrow w_6 = w_7 = w_8 = 0$
   Using Shvab-Zeldovich combinations, to determine the mass fractions and the enthalpy we need to solve two additional equations, for example

$$\begin{aligned} \mathcal{L}_g(Y_V^g) &= f_V^m \text{ on } \Omega_F \\ \mathcal{L}_g(Y_{H_2}^g) &= f_{H_2}^m \text{ on } \Omega_F \end{aligned}$$

   with boundary conditions $Y_V^g = 0$ and $Y_{H_2}^g = 0$ on $\Gamma_F$

# Solid phase model

The mass of a coal particle is determined by:

$$m_p = m_{H_2O} + m_V + m_C + m_{ash}.$$

The evolution of $m_{H_2O}$, $m_V$ and $m_C$, with the radial coordinate $r$ and time $t$, is given by

$$\frac{dm_V}{dt} = -v_p w_4, \quad \frac{dm_{H_2O}}{dt} = -v_p w_5, \quad \frac{dm_C}{dt} = -v_p(w_1 + w_2 + w_3),$$

with $v_p$ the particle volume.
Temperature of the particle is obtained from the equation:

$$m_p c_s \frac{dT_p}{dt} = 4\pi a^2 (q_p'' + q_r'') + \int_0^a \left( \sum_{i=1}^{8} q_i w_i \right) 4\pi r^2 dr,$$

## Heat flux by conduction

$$q_p'' = k \frac{dT}{dr}\Big|_{r=a+}$$

## Heat flux by radiation

$$q_r'' = \varepsilon_p \left( \frac{1}{4} \int_{S^2} I(x,\omega) d\omega - \sigma T_p^4 \right)$$

# Solid phase model

- The model considers simultaneously the char gasification and the processes of moisture evaporation and devolatilization.
- For the generation of volatiles and moisture evaporation we shall use the simple laws

$$w_4 = B_4 e^{-E_4/\mathcal{R}T_p}\rho_V, \; w_5 = B_5 e^{-E_5/\mathcal{R}T_p}\rho_{H_2O}$$

- For the char gasification reactions, Damköhler numbers are defined as

$$\mathrm{Da}_i = (a^2/\mathcal{D}_e)B_i e^{-E_i/\mathcal{R}T_p}, \; i = 1,2,3$$

The activation energies $E_i$ of these reactions are considered large, so:

1. If $\mathrm{Da}_i \ll 1 \Rightarrow$ Kinetically-controlled reactions. Char gasification reactions are considered frozen.
2. If $\mathrm{Da}_i \gg 1 \Rightarrow$ Diffusion-controlled reactions. Very fast reactions of char gasification.

# Solid phase model

For each gasification reaction $i$ we could define a transition temperature $T_{c,i}$ for which $\mathrm{Da}_i = 1$.

So,

1. if $T_p < T_{c,i} \Rightarrow \mathrm{Da}_i < 1$ and the $i$-th reaction considered as frozen,
2. if $T_p > T_{c,i} \Rightarrow \mathrm{Da}_i > 1$ and the $i$-th reaction becomes so fast that it occurs, in a diffusion controlled way, in a thin layer surrounding a shrinking char core.

Advantage:

- The analysis of the gasification reactions depend only on $T_{c,i}$ as a characteristic of the coal, and not on the values of the frequency factor $B_i$ or on the activation energy $E_i$, which depends on the coal type and are not well-known.

For the simulations we will assume that

$$T_{c,i} = T_c, \ i = 1, 2, 3$$

# Solid phase model

When $T_p > T_c$ we distinguish the following cases:

1. **Large particles with high ash content** (BFL).
   The initial particle content of ashes is enough to consider that the outer radius of the particle remains constant. The gas oxidation reactions are fast enough to take place in diffusion flames around or inside the particles.
2. **Small particles with high ash content** (BFLs1).
   Coal particles are smaller than a critical diameter, lower than 100 $\mu$m, for the extinction of the diffusion flame. They have sufficient ash content to maintain a non-swelling shell of ashes, so their radius can be considered constant.
3. **Low ash content particles** (BFLs2).
   The small content of ashes leads to the fragmentation of the porous layer of the particles after the char gasification, so their radius changes along the time.

# Solid phase model

For example, in the case of a small coal particle with high ash content in $\Omega_F$, to determine the char gasification rate ($w_1$ and $w_3$) we have to solve

$$\frac{11}{3}\frac{\lambda_1}{\lambda} = \left\{ Y^g_{CO_2} + \frac{11}{3}\frac{\lambda_1}{\lambda} \right\} e^{\lambda \frac{\mathcal{D}}{\mathcal{D}_e}(1-r_p/r_c)-\lambda},$$

$$\frac{3}{2}\frac{\lambda_3}{\lambda} - \frac{\lambda_5}{\lambda} = \left\{ Y^g_{H_2O} + \frac{3}{2}\frac{\lambda_3}{\lambda} - \frac{\lambda_5}{\lambda} \right\} e^{\lambda \frac{\mathcal{D}}{\mathcal{D}_e}(1-r_p/r_c)-\lambda},$$

with $\lambda_i = \frac{r_p^2}{3\rho\mathcal{D}} w_i$, $i = 1, .., 5$, the nondimensional reaction rates and $\lambda = \lambda_1 + \lambda_3 + \lambda_4 + \lambda_5$.

For the others cases:

## References


- A. Bermúdez, J.L. Ferrín and A. Liñán. *The modelling of the generation of volatiles, $H_2$ and CO, and their simultaneous diffusion controlled oxidation, in pulverized coal furnaces*, Combusion Theory and Modelling, 11(6), 2007
- A. Bermúdez, J.L. Ferrín, A. Liñán and L. Saavedra. *Numerical simulation of group combustion of pulverized coal*, Combustion and Flame, 2011, doi:10.1016/j.combustflame.2011.02.002

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# Particle motion

Velocity of the particle:

$$\frac{d\mathbf{v}_p}{dt} = F_A\left(\mathbf{v}_g - \mathbf{v}_p\right) + \mathbf{g},$$
$$\mathbf{v}_p(0) = \mathbf{v}_{p0},$$

where $F_A$ is the drag force per unit mass,

$$F_A = \frac{3}{16}\frac{\mu}{\rho_p a^2} C_D Re.$$

$Re$: Reynolds relative to the particle

$$Re = \rho_g \mid \mathbf{v}_g - \mathbf{v}_p \mid \frac{2a}{\mu}$$

$C_D$: Drag coefficient

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

# Stochastic particle dispersion

- To take into account the turbulence effect we have coupled the particle motion model with a *discrete random walk model*. The instantaneous fluid velocity is calculated as

$$\mathbf{v}_g = \bar{\mathbf{v}}_g + \left( \xi_1 \sqrt{\frac{k}{\epsilon}}, \xi_2 \sqrt{\frac{k}{\epsilon}}, \xi_3 \sqrt{\frac{k}{\epsilon}} \right)$$

  where $\xi_i, i = 1, 2, 3$ are normally distributed random numbers.
- The random value of the velocity is kept constant over an interval of time given by the characteristic lifetime of the eddies.
- We compute the trajectory, the mass, the temperature and the sources to the gas phase for a sufficient number of representative particles (“number of tries”) with different sizes dropped from each cell of each inlet.

# Outline

# Numerical methods

- The convection-diffusion equations of the gas phase model can be written as

$$\rho \frac{Du}{Dt}(x,t) - \operatorname{div}\left(\left(\mathcal{D}(x,t) + \frac{\mu_t(x,t)}{c_t}\right)\operatorname{grad} u(x,t)\right) + f_m(x,t)u(x,t) = f(x,t),$$

  being $c_t$ a model constant and $\mathcal{D}$ representing the mass diffusion or the molecular viscosity depending on the equation.

- In order to solve them we use Lagrange-Galerkin methods of second order in space and time. These methods are based on the discretization of the material derivative along the characteristic curves

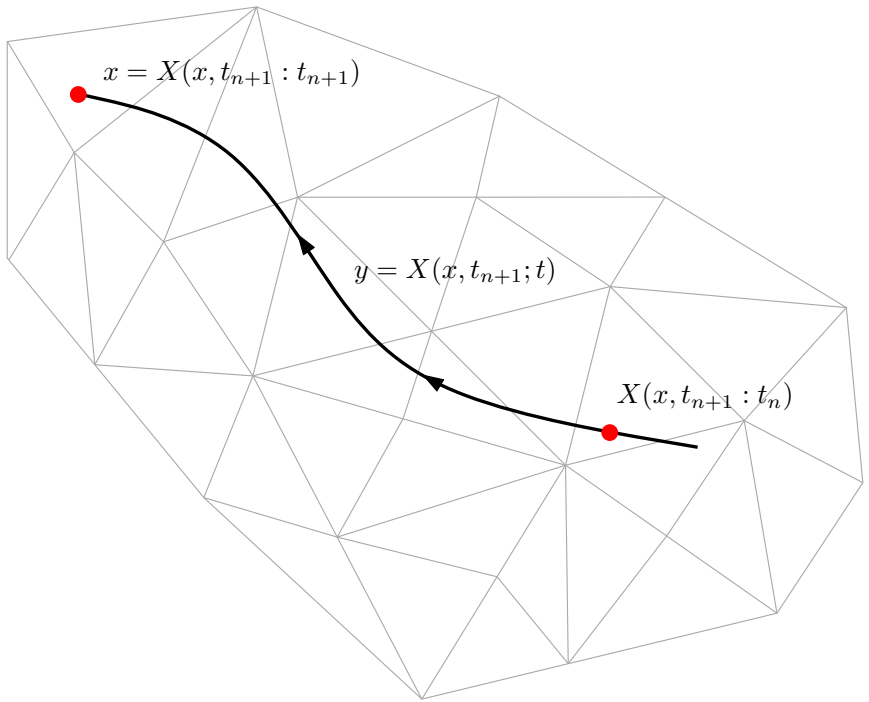
$$\frac{Du}{Dt}(x,t_{n+1}) \approx \frac{1}{2\Delta t}\left(3u^{n+1}(x) - 4(u^n \circ \chi^n)(x) + (u^{n-1} \circ \chi^{n-1})(x)\right),$$

  combined with a Galerkin projection in the framework of finite element methods.

- The characteristic curve $\chi$ is the solution of the initial value problem

$$\begin{cases} \dfrac{d\chi(x,t^{n+1};s)}{ds} = & \mathbf{v}_g(\chi(x,t^{n+1};s),s) \\ \chi(x,t^{n+1};t^{n+1}) = & x \end{cases}$$

The point $\chi^n(x) := \chi(x,t^{n+1};t^n)$, was the position at the instant $t = t^n$ of the fluid particle that is in $x$ at the instant $t^{n+1}$ and that moves with velocity $\mathbf{v}_g$.



Advantages of these methods:

1. The discretization of the material derivative is a natural way to introduce upwinding from the physical point of view.
2. The resulting linear system of equations is symmetric.
3. The method is unconditionally stable if the Galerkin projection is performed exactly, this allows to use large $\Delta t$ in the calculations.

Unfortunately, LG methods have some drawbacks:

1. The calculation of a linear system in every time step, which can have a huge dimension specially in 3D problems.
2. The use of high order quadrature rules in order to maintain the good stability properties of the method. These rules have a significant number of points.
3. The calculation in every iteration of the position of each quadrature point at the previous time step.

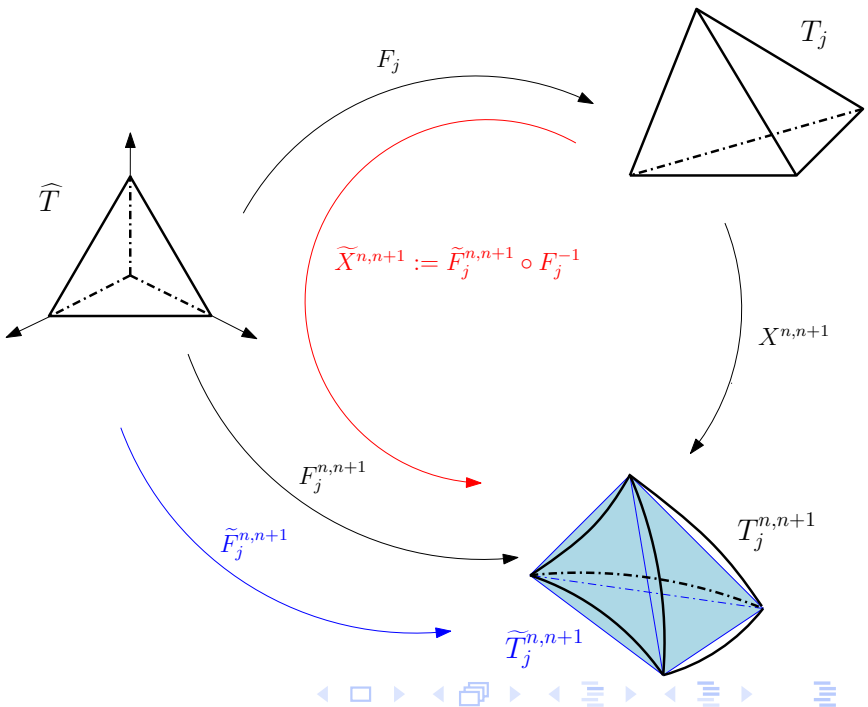
# Numerical methods

To overcome these shortcomings we use:

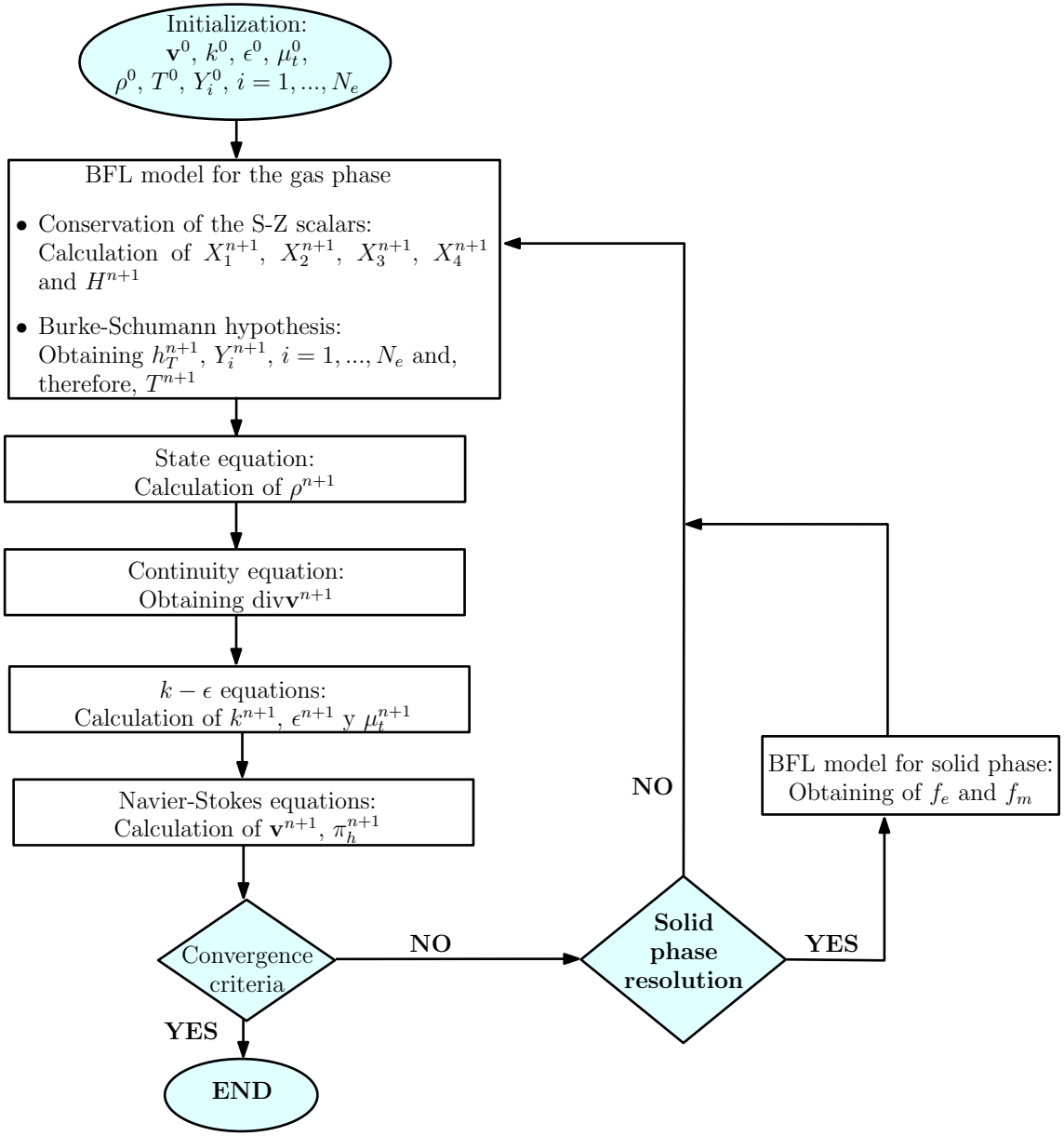
1. Parallelized linear solvers specially designed for Intel processors (MKL library).
2. Modified Lagrange-Galerkin methods (MLG). These methods allow us to compute all the quadrature points at the previous step moving only the mesh vertices. These methods are more efficient (between 15% and 50%) than the convectional ones maintaining the rate of convergence.

## Reference

- R. Bermejo and L. Saavedra *Modified Lagrange-Galerkin methods of first and second order in time for convection-diffusion problems*, Under revision in Numerische Mathematik, 2011.



# Global algorithm



# CFD code

The new models and the numerical methods to solve them have been incorporated to a home made code called SC3D (“Simulación de Calderas en 3D”). This code was designed to simulate industrial furnaces of a Power Plant.

Future version of the code should include:

1. Radiation model.
2. Turbulent formulation of the BFL model.
3. Wall laws.
4. Parallelization.

# Outline

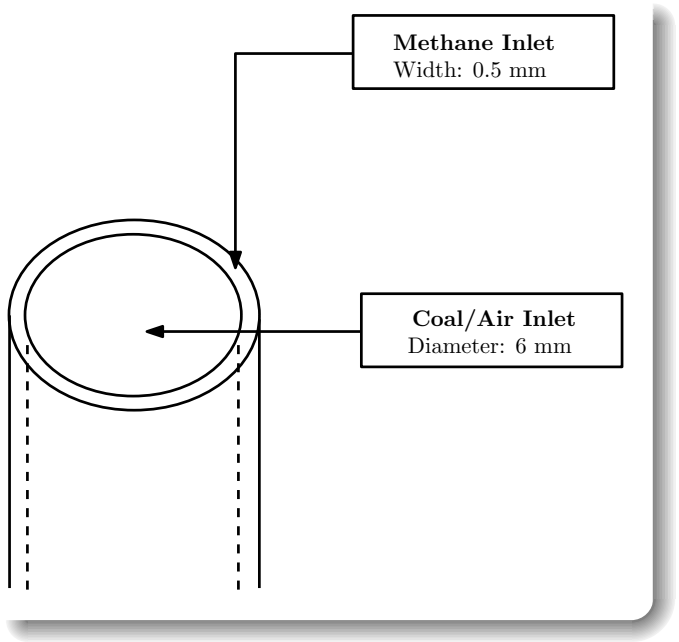
# Simulation of a pulverised coal jet flame

A detailed study of the structure of a turbulent pulverised coal flame has been done in

- Hwang, S., Kurose, R., Akamatsu, F., Tsuji, H., Makino, H. and Katsuki,M. *Observation of detailed structure of turbulent pulverised-coal flame by optical Measurement, (Part 1, Time-averaged measurement of behavior of pulverised-coal particles and flame structure)*, JSME International Journal, 49(4), 2006
- Hwang, S., Kurose, R., Akamatsu, F., Tsuji, H., Makino, H. and Katsuki,M. *Observation of detailed structure of turbulent pulverised-coal flame by optical Measurement, (Part 2, Instantaneous two-dimensional measurement of combustion reaction zone and pulverised coal particles),* JSME International Journal, 49(4), 2006

# Description of the problem

- A laboratory scale burner was specially manufactured to obtain a pulverised coal jet burning with a flame in ambient air.
- Methane is supplied to generate an annular pilot flame needed for the initial heating of the particles to provide the volatiles required for the flame stabilization. The methane flow rate is the minimum needed to form a stable flame.




| Experimental conditions | |
|---|---|
| Air flow rate | $1.80 \times 10^{-4} \mathrm{m}^3/\mathrm{s}$ |
| $CH_4$ flow rate | $2.33 \times 10^{-5} \mathrm{m}^3/\mathrm{s}$ |
| Pulverized coal flow rate | $1.49 \times 10^{-4} \mathrm{kg}/\mathrm{s}$ |

Stages of the experiment:

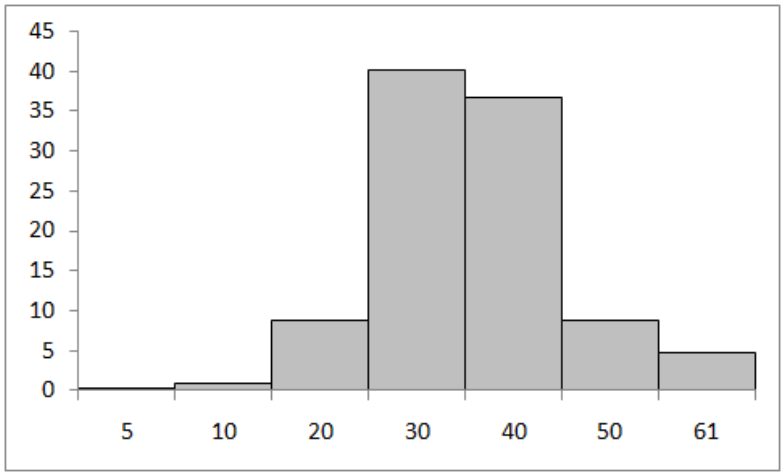
1. The air is supplied to the main burner port and the methane to the annular slit burner. The gas flame due to the air and the methane is formed.
2. When the methane diffusion flame becomes stable the pulverized coal particles are injected.

# Description of the problem

The coal used in the experiment is Newlands bituminous coal.

| Proximate analysis (Dry basis) [wt %] | |
|---|---|
| Volatile matter | 26.9 |
| Fixed carbon | 57.9 |
| Ash | 15.2 |
| **Ultimate analysis (Dry basis) [wt %]** | |
| $C$ | 71.9 |
| $H$ | 4.4 |
| $N$ | 1.58 |
| $O$ | 6.53 |
| $S$ | 0.39 |
| | |
| High heating value | $2.81 \times 10^7\ J/kg$ |
| Density | 1000 $kg/m^3$ |
| Specific heat | 1000 $J/(kgK)$ |

Properties of coal



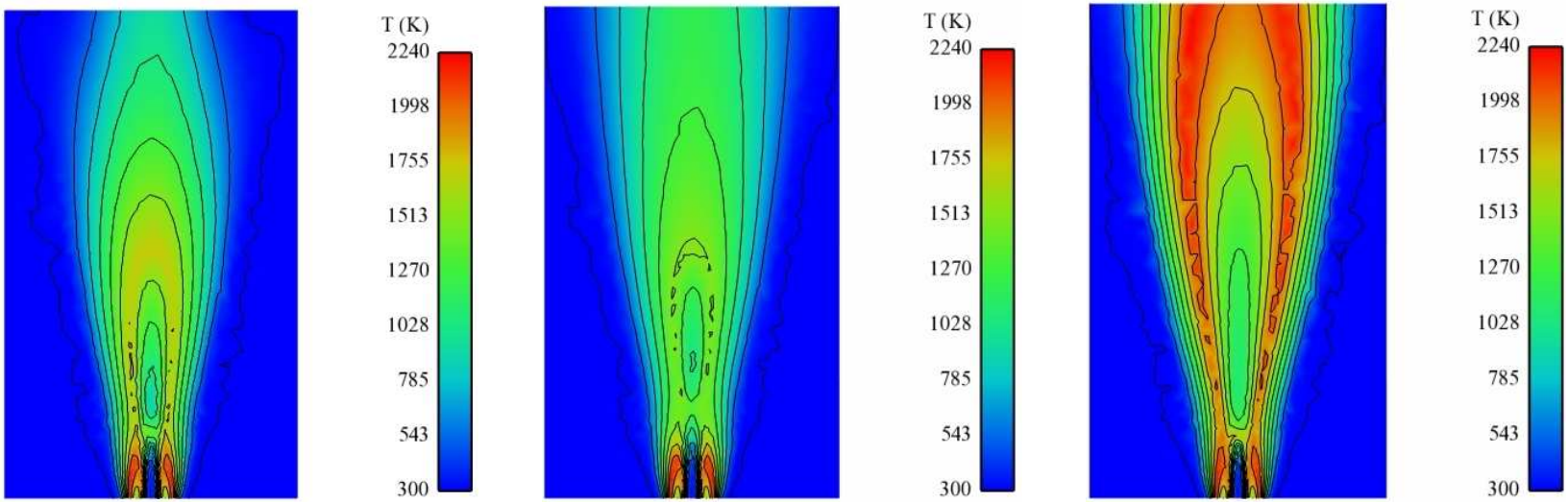

Mass percentage of particles by diameter range

# Simulation of a pulverised coal jet flame

Stages of the simulation:

1. An axisymmetric steady-state simulation of the first stage of the experiment was performed with the commercial code FLUENT version 12.1.4.
2. This simulation has been carried out to calculate profiles for the velocity, the temperature, the composition and the turbulence parameters of the gas mixture near the burner.
3. With these profiles we will carry out three 3D simulations with the different versions of our code corresponding to the three BFL models for the solid phase.
4. The purpose of these simulations is to compare our three models among them and with the experimental data.

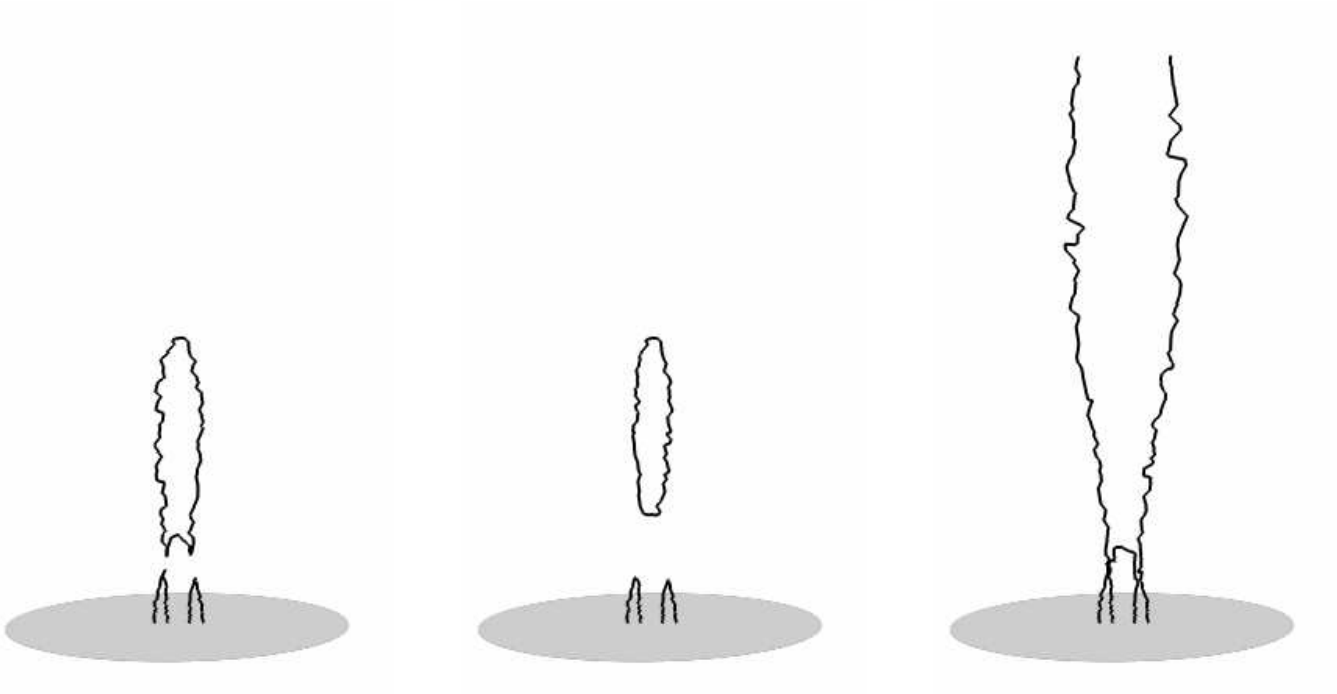
# Comparison of the three BFL models




BFL BFLs1 BFLs2

Contours of temperature (K)

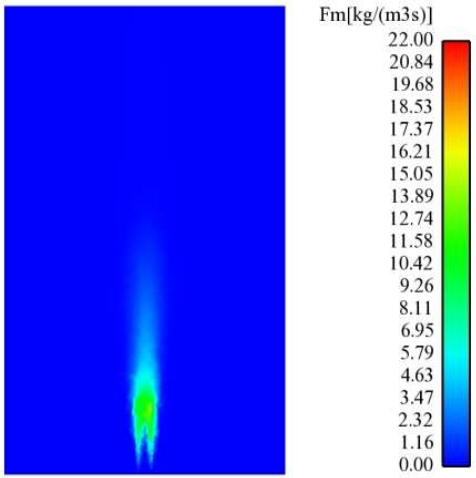
# Comparison of the three BFL models



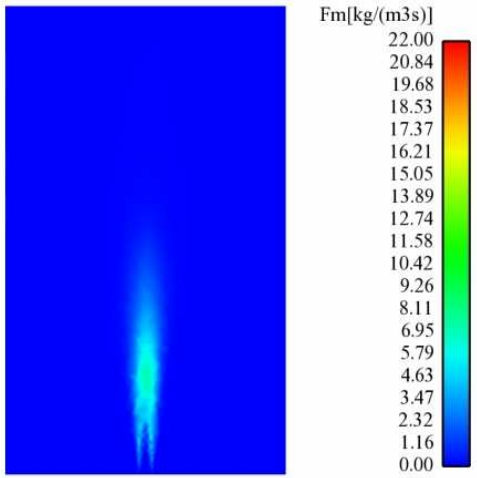
BFL BFLs1 BFLs2

Position of the diffusion flame

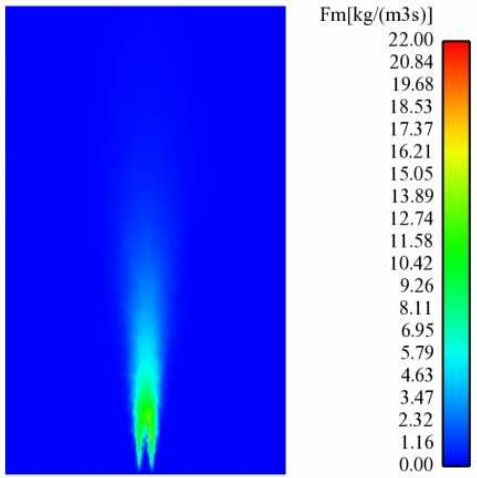
# Comparison of the three BFL models




BFL



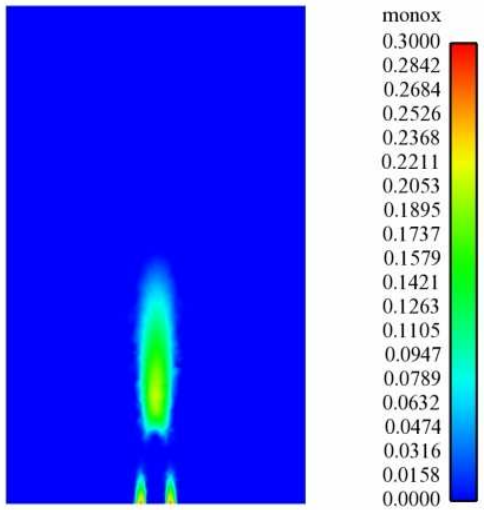

BFLs1



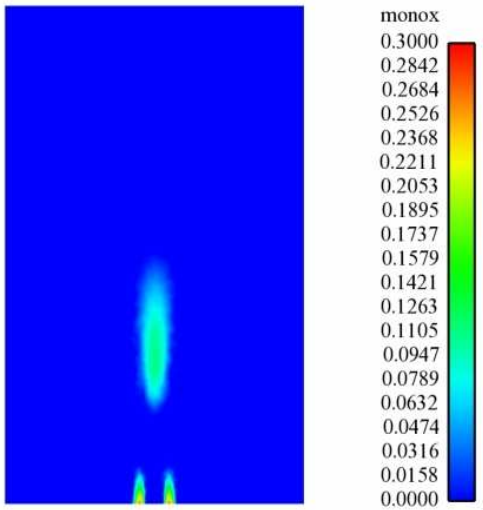

BFLs2

Homogenized mass source $(\mathrm{kg}/(\mathrm{m}^3\mathrm{s}))$

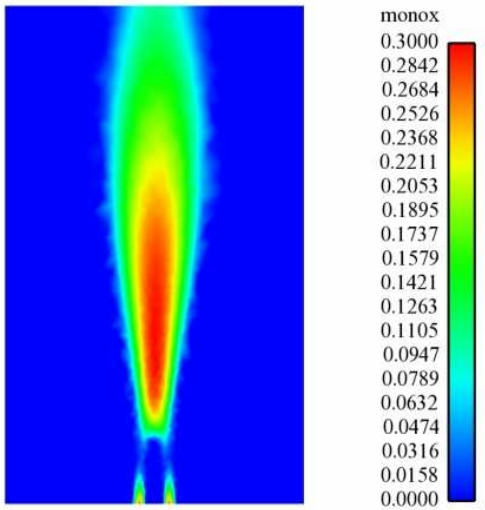
# Comparison of the three BFL models




BFL




BFLs1




BFLs2

Mass fraction of $CO$

# Comparison of the three BFL models

| | Released volatiles (%) | Gasified char (%) |
|---|---|---|
| BFL | 99.99 | 11.87 |
| BFLs1 | 99.99 | 11.51 |
| BFLs2 | 99.99 | 98.49 |
| **Experiment** | 44.6 | 11.3 |

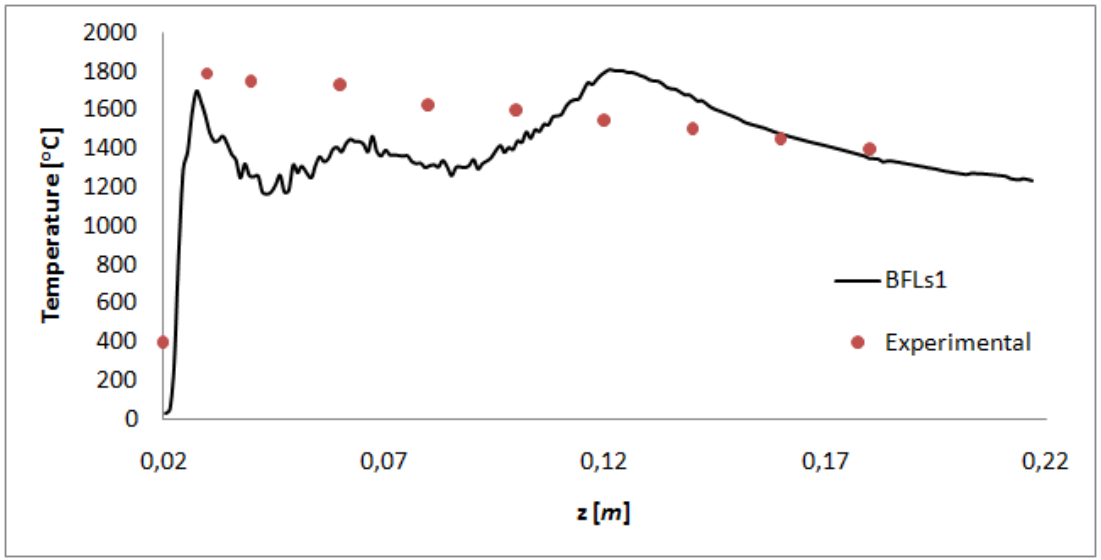
Some comments:

- Our model should be extended to account for the presence of two types of volatiles with different rates of devolatilization.
- In view of these results we can conclude that the BFLs2 model is not appropriate to describe the results of this experiment, and a 15% of ash content cannot be considered as low enough to justify the ash layer disruption.
- Taking into account that the mean diameter of the particles is $33\mu\mathrm{m}$, the BFLs1 is the most suitable model. Therefore we going to compare the results of the simulation done with this model with the experimental results.

# Results of the BFLs1

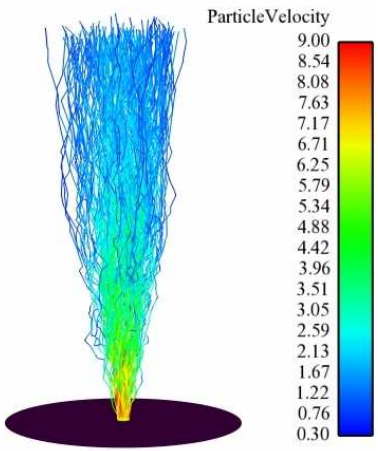
(Cargando Video)

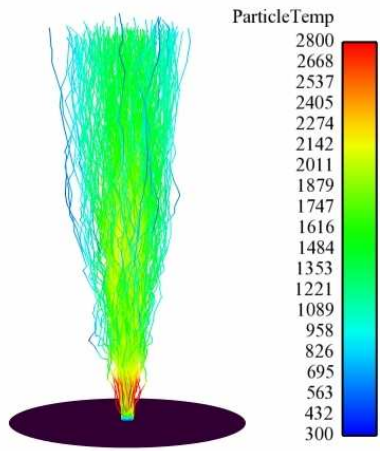
# Results of the BFLs1

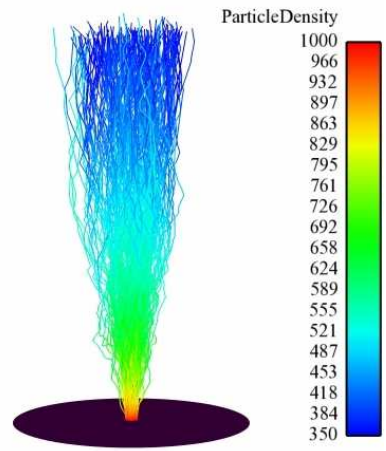



Distribution of particle temperature on the central axis

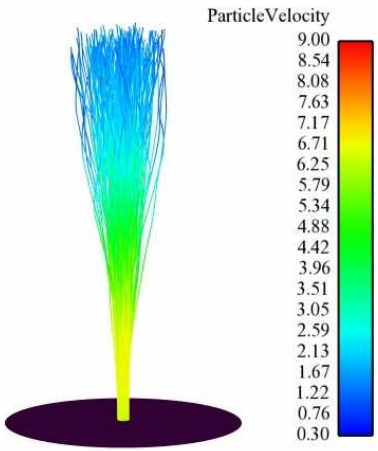
# Results of the BFLs1

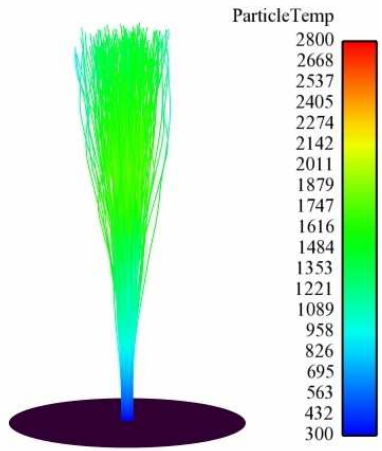


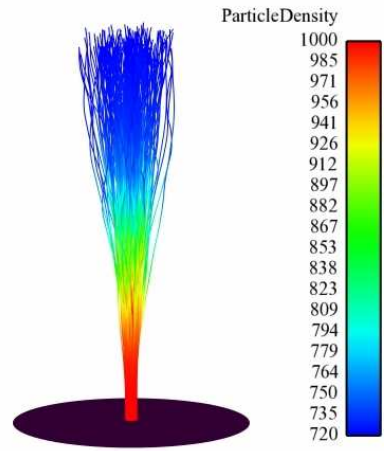




5 $\mu$m diameter particles



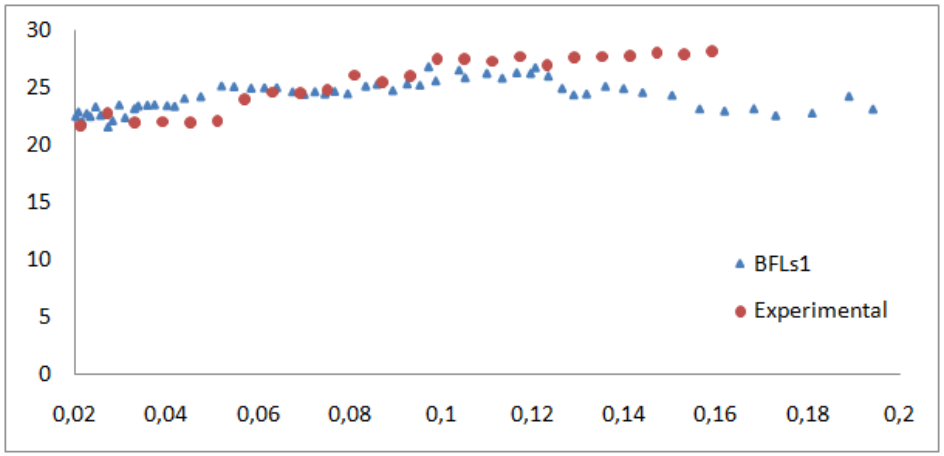




61 $\mu$m diameter particles

Trajectory of coal particles colored by $\mathbf{v}_p$, $T_p$ y $\rho_p$

# Comparison with the experimental data




Distribution of mean diameter on the central axis

We can see:

- Until $z = 120\text{mm}$ the mean diameter is greater the farther you are from the burner. This is because smaller particles are more dispersed and therefore away from the axis.
- From $z = 120\text{mm}$ the mean diameter decreases, unlike the experimental data shows. This fact could be explained because the BFLs1 model does not consider changes in particle sizes and also because turbulent dispersion of the particles is overestimated.

**Thanks for your attention!**