Modelling combustion of coal particles*

A. Bermúdez[1], J.L. Ferrín[1], A. Liñán[2] and O. López[1]

(1) *Departamento de Matemática Aplicada. Universidad de Santiago de Compostela. 15706 Santiago. Spain*
(2) *E.T.S. Ingenieros Aeronáuticos. Universidad Politécnica de Madrid. Spain.*

1 Introduction

The combustion of carbon particles has been the subject of many analytical and empirical research because of the practical utility of this topic with respect to pulverized coal combustion, which is the most widely used method in coal-fired power plants. Two classical pappers by Nusselt [11] and Burke and Schumann [1] can be considered the first important contributions to the field from a theoretical point of view. In the former, it is assumed that oxidation of carbon only takes place at the surface of the particle producing CO and CO_2, depending on the temperature. In the latter, owing to reaction with CO_2 carbon is consumed and then the CO formed reacts with oxigen producing CO_2 at a flame sheet.

More recently Libby and Blake [3] and Libby [2] develop a theory to determine the combustion rate based on the conservation laws for the particle and the surrounding gas. They assume three chemical reactions, two heterogeneous at the surface of the particle and another one homogeneous taking place in the gas phase, in the neighbourhood of the particle. Using the same methodology as Liñán [4], i.e. high activation energy asymptotics, they analyze the limit cases where the homogeneous reaction is either frozen or in

---

*this work has been supported by ENDESA (As Pontes, A Coruña, Spain) under contract

equilibrium.
Transition between the two situations have also been analyzed in Matalon [8], [9] and [10]. In Makino and Law [7] an ignition criterion for the CO flame is obtained. Finally, approximated explicit expressions for the combustion rate are obtained by Makino [6].
In the present paper we recall the models obtained in Libby and Blake [3] and then we do mathematical analysis to show existence of solution. We also solve them numerically and compare the computed solution to those obtained when some approximated explicit solutions are considered.

2 The combustion model

We consider a simplified kinetic model consisting of the three following chemical reactions:

- Carbon oxidation by carbon dioxide

$$CO_2 + C \to 2\ CO + (q_1) \tag{2.1}$$

- Carbon oxidation by oxygen

$$\frac{1}{2}O_2 + C \to CO + (q_2) \tag{2.2}$$

- Carbon monoxide oxidation by oxygen

$$CO + \frac{1}{2}\ O_2 \to CO_2 + (q_3) \tag{2.3}$$

where q_i, $i = 1, 3$ denote the heat of the reaction i per unit of mass of carbon ($i = 1, 2$) and carbon monoxide ($i = 3$).

The first two reactions take place on the surface of the particle while the third one can occur either on the surface of the particle or in the gas next to it, depending on the oxygen and carbon monoxide local concentrations in the gas environment. We analyze the two limiting cases of infinitely fast and frozen gas-phase reaction (2.3).

3 Modelling the gas-phase

In this section we suppose reaction (2.3) takes place in the gas-phase very close to the particle under consideration. If we restrict our attention to the case of low Peclet number, based on the relative velocity of the particle to the local gas environment, then the effect of this ambient gas on the particle may be neglected and the particle and the surrounding concentration and temperature fields be considered spherico-symmetrical. Let indices 1, 2 and 3 denote the species CO_2, O_2 and CO respectively. In spherical coordinates the conservation equations for the gas-phase are the following

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \rho v) &= 0 && (3.1)\\ \rho \frac{\partial Y_\alpha}{\partial t} + \rho v \frac{\partial Y_\alpha}{\partial r} - \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \rho D \frac{\partial Y_\alpha}{\partial r}) &= s_\alpha w_3 && (3.2)\\ \rho c \frac{\partial T}{\partial t} + \rho v c \frac{\partial T}{\partial r} - \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 k \frac{\partial T}{\partial r}) &= q_3 w_3 && (3.3) \end{aligned}$$

where v is the radial velocity, Y_α the mass fraction of species α, T is the temperature, w_3 is the mass combustion rate per unit volume of species 3 due to the chemical reaction (2.3) taking place in the gas-phase, s_α, $\alpha = 1, 2, 3$ are stoichiometric coefficients relating the mass production rate of species α to w_3, D is a diffusion coefficient which is supposed to be the same for all species, c is the specific heat and k the thermal conductivity of the gas.

From the momentum equations we can estimate the spatial variations of pressure in the flow field around the particle. It turns out to be so small that in the equation of state for the gas mixture we can replace p by its value p_g in the gas environment far from the particle. If we consider the gas to be a mixture of perfect gases the equation of state becomes

$$p_g = \rho \mathcal{R} T / M \tag{3.4}$$

where M is the molecular mass of the mixture, i.e.

$$\frac{1}{M} = \Sigma_\alpha \frac{Y_\alpha}{M_\alpha} \tag{3.5}$$

and $\mathcal{R}$ is the universal gas constant.

We adopt the following expressions for w_α (see for instance [3]):

$$w_3 = \rho^2 Y_2^{1/2} Y_3 B_3 e^{-E_3/\mathcal{R}T} \tag{3.6}$$

As usual B_3 denotes a frequency factor which is proportional to $Y_{H_2O}^{1/2}$ (the reaction is catalyzed by water vapor) and E_3 the activation energy for reaction (2.3).

4 Quasi-steady gas-phase model

An asymptotic analysis similar to that in Liñan[5] shows that the characteristic response time of the gas phase at a distance r from the center of the particle of the order of δ_p (the radius of the particle), is short compared to the change in boundary conditions at the moving interface $r = \delta_p$. This allows us to use the quasi-steady state approximation in the analysis of the gas-phase response, that is, to neglect the time derivatives in equations (3.1)-(3.3). Thus they can be written as follows:

$$\rho v r^2 = \dot{m} \tag{4.1}$$

$$\frac{\dot{m}}{r^2}\frac{dY_1}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \rho D \frac{dY_1}{dr}) = \frac{11}{7} w_3 \tag{4.2}$$

$$\frac{\dot{m}}{r^2}\frac{dY_2}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \rho D \frac{dY_2}{dr}) = \frac{-4}{7} w_3 \tag{4.3}$$

$$\frac{\dot{m}}{r^2}\frac{dY_3}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \rho D \frac{dY_3}{dr}) = -w_3 \tag{4.4}$$

$$\frac{\dot{m}}{r^2}\frac{dT}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \frac{k}{c} \frac{dT}{dr}) = \frac{q_3}{c} w_3 \tag{4.5}$$

where $4\pi\dot{m}$ denotes the carbon rate of combustion due to the surface reactions (2.1) and (2.2). These equations, which hold for $r > \delta_p$, have to be integrated for the following boundary conditions:

- At $r \to \infty$

$$Y_\alpha = Y_{\alpha g} \text{ for } \alpha = 1, 2, 3 \tag{4.6}$$

$$T = T_g \tag{4.7}$$

  where index g stands for values of fields in the ambient gas at the position of the particle under consideration.

- At the surface of the particle: $r = \delta_p$

$$Y_\alpha = Y_{\alpha s}, \text{ for } \alpha = 1, 2, 3 \tag{4.8}$$

$$\begin{aligned} T &= T_p && (4.9)\\ \dot{m}Y_1 - r^2\rho D \frac{dY_1}{dr}_{|r=\delta_p} &= -\frac{11}{3}\dot{m}_1 && (4.10)\\ \dot{m}Y_2 - r^2\rho D \frac{dY_2}{dr}_{|r=\delta_p} &= -\frac{4}{3}\dot{m}_2 && (4.11)\\ \dot{m}Y_3 - r^2\rho D \frac{dY_3}{dr}_{|r=\delta_p} &= \frac{14}{3}\dot{m}_1 + \frac{7}{3}\dot{m}_2 && (4.12)\\ \dot{m}cT - r^2 k \frac{dT}{dr}_{|r=\delta_p} &= \dot{m}cT_p - \delta_p^2 q_g && (4.13) \end{aligned}$$

where $\dot{m}_1$ and $\dot{m}_2$ denote the carbon reaction rate due to surface reactions (2.1) and (2.2), T_p denotes the temperature of the particle and q_g is the heat flux coming to the particle by conduction from the gas. We have

$$\dot{m} = \dot{m}_1 + \dot{m}_2 \qquad (4.14)$$

$$q_g = k\frac{dT}{dr}_{|r=\delta_p} \qquad (4.15)$$

5 Infinitely fast gas-phase reaction

5.1 Separated flame sheet

Solving this system of differential equations is not an easy task. However the problem becomes much simpler in some limit cases. In what follows we shall describe the process in the limit of infinite Damkohler number for the gas-phase reaction. In this limit the reactants cannot coexist because equations (3.6), (4.3) and (4.4) imply

$$Y_2 Y_3 = 0 \qquad (5.16)$$

Then the chemical reaction is confined to an infinitely thin reaction zone, or flame sheet, at $r = r_f$, separating an interior region without oxygen and an outer region free from carbon monoxide.

The reactants reach the reaction zone at stoichiometric proportions from both sides by diffusion and the production terms in equations (4.3)-(4.5) become Dirac delta measures.

This diffusion-controlled model results from a direct use of the Burke-Schumann analysis of diffusion flames for infinitely fast reactions.

On the other hand, to be coherent with the assumption of infinitely fast gas-phase reaction we will take $Y_{3g} = 0$ in this section.
Now we use the classical linear combinations of equations (4.3)-(4.5) showing that the Shvab-Zeldovich coupling functions follow the same conservation equations as a passive scalar, i.e.

$$\begin{aligned} \frac{\dot{m}}{r^2}\frac{d}{dr}(Y_3 - \frac{7}{4}Y_2) - \frac{1}{r^2}\frac{d}{dr}\{r^2\rho D\frac{d}{dr}(Y_3 - \frac{7}{4}Y_2)\} &= 0 \qquad (5.17)\\ \frac{\dot{m}}{r^2}\frac{d}{dr}(Y_1 + \frac{11}{4}Y_2) - \frac{1}{r^2}\frac{d}{dr}\{r^2\rho D\frac{d}{dr}(Y_1 + \frac{11}{4}Y_2)\} &= 0 \qquad (5.18)\\ \frac{\dot{m}}{r^2}\frac{d}{dr}(\frac{cT}{q_3} + \frac{7}{4}Y_2) - \frac{1}{r^2}\frac{d}{dr}\{r^2\rho D\frac{d}{dr}(\frac{cT}{q_3} + \frac{7}{4}Y_2)\} &= 0 \qquad (5.19)\end{aligned}$$

On the other hand, as already mentioned, the infinite Damkohler number assumption implies

$$\begin{aligned} Y_2 &= 0 \text{ in } r \le r_f \qquad (5.20)\\ Y_3 &= 0 \text{ in } r \ge r_f\ . \qquad (5.21)\end{aligned}$$

Notice that, as a consequence of (5.20), if $\delta_p < r_f$ then the heterogeneous reaction (2.2) cannot take place. Then $\dot{m}_2 = 0$ and $\dot{m} = \dot{m}_1$.
By integrating equations (5.17)-(5.19) once in r and considering the flux boundary conditions (4.10)-(4.13) at $r = \delta_p$ we obtain

$$\begin{aligned} \dot{m}(Y_3 - \frac{7}{4}Y_2) - r^2\rho D\frac{d}{dr}(Y_3 - \frac{7}{4}Y_2) &= \frac{14}{3}\dot{m} \qquad (5.22)\\ \dot{m}(Y_1 + \frac{11}{4}Y_2) - r^2\rho D\frac{d}{dr}(Y_1 + \frac{11}{4}Y_2) &= -\frac{11}{3}\dot{m} \qquad (5.23)\\ \dot{m}(cT + \frac{7}{4}Y_2q_3) - r^2\rho D\frac{d}{dr}(cT + \frac{7}{4}Y_2q_3) &= \dot{m}cT_p - \delta_p^2q_g \qquad (5.24)\end{aligned}$$

This system has to be integrated once again by using boundary conditions (4.6)-(4.9). First we make only use of those at $r = \infty$ to get

$$\begin{aligned} Y_3 - \frac{7}{4}Y_2 &= \frac{14}{3} + (-\frac{7}{4}Y_{2g} - \frac{14}{3})e^{-\lambda\delta_pLe/r} \qquad (5.25)\\ Y_1 + \frac{11}{4}Y_2 &= -\frac{11}{3} + (\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g})e^{-\lambda\delta_pLe/r} \qquad (5.26)\\ cT + \frac{7}{4}Y_2q_3 &= cT_p - \frac{\delta_p^2q_g}{\dot{m}} + \{c(T_g - T_p)\\ &+ \frac{7}{4}Y_{2g}q_3 + \frac{\delta_p^2}{\dot{m}}q_g\}e^{-\lambda\delta_p/r} \qquad (5.27)\end{aligned}$$

where we have denoted by λ the nondimensional combustion rate defined by

$$\lambda = \frac{\dot{m}c}{k\delta_p}. \tag{5.28}$$

and by Le the Lewis number

$$Le = \frac{k}{\rho c D} \tag{5.29}$$

Then we use boundary conditions at $r = \delta_p$. Thus equations (5.26)-(5.27) lead to expressions giving λ and q_g

$$\lambda = \frac{1}{Le} ln\{(\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g})/(\frac{11}{3} + Y_{1s})\} \tag{5.30}$$

$$q_g = \frac{k}{\delta_p}\{(T_g - T_p) + \frac{7}{4}\frac{Y_{2g}q_3}{c}\}\frac{\lambda}{e^{\lambda} - 1} \tag{5.31}$$

because $Y_2 = 0$ at $r = \delta_p$. On the other hand equation (5.25) enables us to determine the flame location r_f as follows: at $r = r_f$ we must have $Y_2 = Y_3 = 0$ and hence

$$e^{\lambda\delta_p Le/r_f} = 1 + \frac{3}{8}Y_{2g}. \tag{5.32}$$

from which r_f can be obtained.
Let λ_c be defined by

$$\lambda_c = \frac{1}{Le} ln(1 + \frac{3}{8}Y_{2g}). \tag{5.33}$$

Notice that, apart from the Lewis number, λ_c only depends on the oxygen concentration of the ambient gas.
Then for $\lambda < \lambda_c$ we have $r_f < \delta_p$ from (5.32), which is impossible. This corresponds to the case where the three reactions (2.1)-(2.3) take place on the surface of the particle, which will be analyzed later.
If $\lambda > \lambda_c$ we may obtain from (5.27) the temperature of the flame

$$T_f = T_p - \frac{\delta_p^2 q_g}{\dot{m}c} + \{T_g - T_p + \frac{1}{c}(\frac{7}{4}Y_{2g}q_3 + \frac{\delta_p^2}{\dot{m}}q_g)\}/(1 + \frac{3}{8}Y_{2g}) \tag{5.34}$$

and from (5.25) the following expressions for Y_2 and Y_3:

$$Y_2 = -\frac{8}{3} + (\frac{8}{3} + Y_{2g})e^{-\lambda\delta_p Le/r} \text{ if } r > r_f \tag{5.35}$$

$$Y_3 = \frac{14}{3} - (\frac{14}{3} + \frac{7}{4}Y_{2g})e^{-\lambda\delta_p Le/r} \text{ if } r < r_f \tag{5.36}$$

The two equations (5.30) and (5.31) have five unknowns T_p, δ_p, Y_{1s}, λ and q_g. To get a closed system we have to add the equations corresponding to mass and energy balance and chemical kinetics on the surface of the particle, namely

$$
\begin{aligned}
\rho_p \frac{d(\frac{4}{3}\pi\delta_p^3)}{dt} &= -4\pi\dot{m} && (5.37)\\
\frac{4}{3}\pi\delta_p^3\rho_p c_p \frac{dT_p}{dt} &= 4\pi\delta_p^2 q_p + 4\pi\delta_p^2\epsilon(\frac{1}{4}\int_S I(\omega)dS(\omega) - \sigma T_p^4) && (5.38)\\
q_g &= q_p - \frac{1}{\delta_p^2}(q_1\dot{m}_1 + q_2\dot{m}_2) && (5.39)\\
\dot{m}_1 &= \delta_p^2 B_1 e^{-E_1/\mathcal{R}T_p}\rho Y_{1s} && (5.40)\\
\dot{m}_2 &= \delta_p^2 B_2 e^{-E_2/\mathcal{R}T_p}\rho Y_{2s} && (5.41)
\end{aligned}
$$

where ρ_p and c_p denote density and specific heat of the particle, respectively, q_p is the total heat flux to the particle, ϵ is emissivity, σ is the Stephan-Boltzmann constant and $I(\omega)$ is the radiation intensity in the direction ω at the position of the particle.

Recall that, since $\lambda > \lambda_c$ oxygen is completely consumed by the gas-phase reaction at $r = r_f$ and hence $\dot{m}_2 = 0$.

From the whole system (5.30), (5.31) and (5.37)-(5.41) we finally get

$$
\begin{aligned}
\delta_p \frac{d\delta_p}{dt} &= -\lambda \frac{k}{\rho_p c} && (5.42)\\
\lambda &= \mathcal{K}_1 F_1(\lambda) && (5.43)\\
\frac{\delta_p}{3}\rho_p c_p \frac{dT_p}{dt} &= \frac{k}{\delta_p}(T_g - T_p)\frac{\lambda}{e^{\lambda}-1} \\
&+ \frac{k}{\delta_p c}(\frac{7}{4}Y_{2g}q_3\frac{\lambda}{e^{\lambda}-1} + q_1\lambda) \\
&+ \epsilon(\frac{1}{4}\int_S I(\omega)dS(\omega) - \sigma T_p^4) && (5.44)
\end{aligned}
$$

where $\mathcal{K}_1$ and $F_1(\lambda)$ are given by

$$
\begin{aligned}
\mathcal{K}_1 &= B_1 e^{-\frac{E_1}{\mathcal{R}T_p}}\frac{\rho_g T_g}{T_p}\frac{\delta_p c}{k} && (5.45)\\
F_1(\lambda) &= -\frac{11}{3} + \left(\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g}\right)e^{-\lambda Le}. && (5.46)
\end{aligned}
$$

We have made use of the fact that

$$\rho T_p = \rho_g T_g, \tag{5.47}$$

which follows from the state equation (3.4).

5.2 Contiguous flame sheet

In this section we consider the case where $\lambda < \lambda_c$ as defined by (5.28) and (5.33). This corresponds to the three reactions (2.1)-(2.3) taking place on the surface of the particle. We still assume the reaction (2.3) to be infinitely fast.

In this case the gas-phase equations become

$$\rho v r^2 = \dot{m} \tag{5.48}$$

$$\frac{\dot{m}}{r^2}\frac{dY_1}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \rho D \frac{dY_1}{dr}) = 0 \tag{5.49}$$

$$\frac{\dot{m}}{r^2}\frac{dY_2}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \rho D \frac{dY_2}{dr}) = 0 \tag{5.50}$$

$$\frac{\dot{m}}{r^2}\frac{dT}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2 \frac{k}{c} \frac{dT}{dr}) = 0 \tag{5.51}$$

because no reactions take place in the gas. On the other hand boundary conditions are

- At $r \to \infty$

$$Y_\alpha = Y_{\alpha g} \text{ for } \alpha = 1, 2 \tag{5.52}$$

$$T = T_g \tag{5.53}$$

- At the surface of the particle: $r = \delta_p$

$$Y_\alpha = Y_{\alpha s}, \text{ for } \alpha = 1, 2, 3 \tag{5.54}$$

$$T = T_p \tag{5.55}$$

$$\dot{m} Y_1 - r^2 \rho D \frac{dY_1}{dr}_{|r=\delta_p} = \frac{11}{3}(\dot{m}_1 + \dot{m}_2) \tag{5.56}$$

$$\dot{m} Y_2 - r^2 \rho D \frac{dY_2}{dr}_{|r=\delta_p} = -\frac{8}{3}(\dot{m}_1 + \dot{m}_2) \tag{5.57}$$

$$\dot{m} c T - r^2 k \frac{dT}{dr}_{|r=\delta_p} = \dot{m} c T_p - \delta_p^2 q_g \tag{5.58}$$

A first integration of equations (5.48)-(5.51) with boundary conditions (5.55)-(5.58) gives

$$\begin{aligned} \dot{m}Y_1 - r^2\rho D\frac{d}{dr}Y_1 &= \frac{11}{3}\dot{m} && (5.59)\\ \dot{m}Y_2 - r^2\rho D\frac{d}{dr}Y_2 &= -\frac{8}{3}\dot{m} && (5.60)\\ \dot{m}cT - r^2k\frac{d}{dr}T &= \dot{m}cT_p - \delta_p^2 q_g && (5.61) \end{aligned}$$

A second integration taking boundary conditions at infinity into account leads to

$$\begin{aligned} Y_1 &= \frac{11}{3} + (-\frac{11}{3} + Y_{1g})e^{-\lambda\delta_p Le/r} && (5.62)\\ Y_2 &= -\frac{8}{3} + (Y_{2g} + \frac{8}{3})e^{-\lambda\delta_p Le/r} && (5.63)\\ T &= T_p - \frac{\delta_p^2 q_g}{\dot{m}c} + \{T_g - T_p + \frac{\delta_p^2}{\dot{m}c}q_g\}e^{-\lambda\delta_p/r} && (5.64) \end{aligned}$$

In particular, at the surface of the particle we obtain the values of Y_{1s} and Y_{2s} given by

$$\begin{aligned} Y_{1s} &= \frac{11}{3} + (-\frac{11}{3} + Y_{1g})e^{-\lambda Le} && (5.65)\\ Y_{2s} &= -\frac{8}{3} + (Y_{2g} + \frac{8}{3})e^{-\lambda Le} && (5.66) \end{aligned}$$

Notice that $Y_{2s} \geq 0$ if and only if $\lambda \leq \lambda_c$ which is in agreement with the previous analysis for a separated flame sheet. In particular, Y_{2s} corresponds to $\lambda = \lambda_c$.
These expressions are to be replaced in equations (5.40) and (5.41) for $\dot{m}_1$ and $\dot{m}_2$ while the heat flux to the gas phase is now given by

$$q_g = q_p - \frac{1}{\delta_p^2}\{q_1\dot{m}_1 + q_2\dot{m}_2 + q_3(\frac{14}{3}\dot{m}_1 + \frac{7}{3}\dot{m}_2)\}. \qquad (5.67)$$

Now, we can write equations for T_p, δ_p, Y_{1s}, Y_{2s}, λ and q_g. They are (5.65), (5.66) and the following ones:

$$\delta_p\frac{d\delta_p}{dt} = -\lambda\frac{k}{\rho_p c} \qquad (5.68)$$

$$\begin{aligned}
\lambda &= \lambda_1 + \lambda_2 & (5.69)\\
\lambda_i &= \mathcal{K}_i F_i(\lambda)\ i = 1, 2 & (5.70)\\
\frac{\delta_p}{3}\rho_p c_p \frac{dT_p}{dt} &= \frac{k}{\delta_p}(T_g - T_p)\frac{\lambda}{e^{\lambda} - 1} + \frac{k}{\delta_p c}\{(\frac{14}{3}q_3 + q_1)\lambda_1 & \\
&+ (\frac{7}{3}q_3 + q_2)\lambda_2\} + \epsilon(\frac{1}{4}\int_S I(\omega)dS(\omega) - \sigma T_p^4) & (5.71)
\end{aligned}$$

where $\mathcal{K}_1$ is given by (5.45),

$$F_1(\lambda) = \frac{11}{3} + \left(-\frac{11}{3} + Y_{1g}\right) e^{-\lambda Le} \tag{5.72}$$

and $\mathcal{K}_2$ and $F_2(\lambda)$ are given by

$$\begin{aligned}
\mathcal{K}_2 &= B_2 e^{-\frac{E_2}{\mathcal{R}T_p}} \frac{\rho_g T_g}{T_p} \frac{\delta_p c}{k} & (5.73)\\
F_2(\lambda) &= -\frac{8}{3} + \left(\frac{8}{3} + Y_{2g}\right) e^{-\lambda Le}. & (5.74)
\end{aligned}$$

5.3 Mathematical analysis

In this section we prove the existence of solution for the model we have obtained in the previous section. In a first step we study the nonlinear equation giving λ. To begin with, notice that equation (5.43) may be included in (5.70) by defining functions F_1 and F_2 as follows:

$$F_1(\lambda) = \begin{cases} \frac{11}{3} + \left(Y_{1g} - \frac{11}{3}\right) e^{-\lambda Le} & \text{if } \lambda \leq \lambda_c \\ -\frac{11}{3} + \left(\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g}\right) e^{-\lambda Le} & \text{if } \lambda \geq \lambda_c \end{cases} \tag{5.75}$$

$$F_2(\lambda) = \begin{cases} -\frac{8}{3} + \left(\frac{8}{3} + Y_{2g}\right) e^{-\lambda Le} & \text{if } \lambda \leq \lambda_c \\ 0 & \text{if } \lambda \geq \lambda_c \end{cases} \tag{5.76}$$

Then we prove the

Lemma 5.1 *Functions F_1 and F_2 are continuous.*

Figure 1: Function $F_1(\lambda)$

Proof. It is enough to see that for $\lambda = \lambda_c$ the asigned values to F_1 and F_2 are the same. Indeed, notice that if $\lambda = \lambda_c$ then

$$Y_{2g} = \frac{8}{3}(e^{\lambda_c Le} - 1) \tag{5.77}$$

and hence

$$-\frac{11}{3} + \left(\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g}\right) e^{-\lambda_c Le} = \frac{11}{3} + \left(Y_{1g} - \frac{11}{3}\right) e^{-\lambda_c Le}. \tag{5.78}$$

On the other hand we have

$$-\frac{8}{3} + \left(\frac{8}{3} + Y_{2g}\right) e^{-\lambda_c Le} = 0 \tag{5.79}$$

which completes the proof.□

Curves $\mu = F_1(\lambda)$ and $\mu = F_2(\lambda)$ are represented on the $\lambda - \mu$ plane in figures 1 and 2, for $Y_{1g} = 0.11$ and $Y_{2g} = 0.13$. In this case $\lambda_c = 0.06019$.

For the sake of simplicity we denote by G the function defined by

$$G(\lambda) = \mathcal{K}_1 F_1(\lambda) + \mathcal{K}_2 F_2(\lambda). \tag{5.80}$$

Figure 2: Function $F_2(\lambda)$

Now we prove the existence of a positive solution for the equation

$$\lambda = G(\lambda) \tag{5.81}$$

giving λ. As coefficents $\mathcal{K}_1$ and $\mathcal{K}_2$ are always positive, we have the following

Proposition 5.1 *There exists* $\lambda \in [0, 1/Le)$*, positive solution of the equation (5.81).*

Proof. Notice that if $(\overline{\lambda}, \overline{\mu})$ is an intersection point of the lines $\mu = \lambda$ and $\mu = G(\lambda)$ then $\overline{\lambda}$ is a solution of (5.81).
On the other hand $F_1(0) = Y_{1g}$ and $F_2(0) = Y_{2g}$ hence

$$G(0) \geq 0. \tag{5.82}$$

Furthermore, since $\lambda_c < 1$ we have

$$G(1/Le) = \mathcal{K}_1\{-\frac{11}{3} + \left(\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g}\right)e^{-1}\} < 0 \tag{5.83}$$

so the two lines must intersect at some $(\overline{\lambda}, \overline{\mu})$ with $\overline{\lambda} \in [0, 1/Le)$.□

Now we deal with the energy equation which can have the two forms (5.44) or (5.71) depending on whether $\lambda \leq \lambda_c$ or not. It is not difficult to see

that for $\lambda = \lambda_c$ the right hand sides of these two equations coincide.
Indeed, it is enough to use continuity of F_1, the fact that $F_2(\lambda_c) = 0$ and the equality

$$\frac{7}{4} Y_{2g} \frac{1}{e^{\lambda_c Le} - 1} = \frac{14}{3}. \tag{5.84}$$

which follows from (5.33).

5.4 An approximated explicit expression for the combustion rate

The mathematical model introduced in the previous sections involves the nonlinear equation (5.81) which needs using an iterative algorithm for numerical solution. In this section we obtain an approximation leading to a linear eqution. It is based on the fact that in many practical situations $\lambda Le \ll 1$ and then

$$e^{-\lambda Le} \sim 1 - \lambda Le \tag{5.85}$$

By replacing this approximation in (5.75) and (5.76) we get the following approximated expressions for F_1 and F_2

$$\hat{F}_1(\lambda) = \begin{cases} \frac{11}{3} + \left(Y_{1g} - \frac{11}{3} \right) (1 - \lambda Le) & \text{for contiguous flame} \\ -\frac{11}{3} + \left(\frac{11}{3} + Y_{1g} + \frac{11}{4} Y_{2g} \right) (1 - \lambda Le) & \text{for separated flame} \end{cases} \tag{5.86}$$

$$\hat{F}_2(\lambda) = \begin{cases} -\frac{8}{3} + \left(\frac{8}{3} + Y_{2g} \right) (1 - \lambda Le) & \text{for contiguous flame} \\ 0 & \text{for separated flame} \end{cases} \tag{5.87}$$

Now we have to give a criterion to distinguish between the two cases of contiguous and separated flame sheet. For this we first write the equation (5.32)

$$(1 + \frac{3}{8} Y_{2g}) e^{-\lambda Le \frac{\delta_p}{r_f}} = 1 \tag{5.88}$$

and use approximation (5.86). Then the limit case $\delta_p = r_f$ corresponds to

$$\lambda_c = \frac{1}{Le} (1 - \frac{1}{1 + \frac{3}{8} Y_{2g}}) \tag{5.89}$$

It is not difficult to see that this choice guarantees continuity of functions $\hat{F}_1$ and $\hat{F}_2$.
By replacing these approximations in (5.43), (5.69) and (5.70) we get the following explicit values for λ:

$$\lambda = \frac{\mathcal{K}_1 Y_{1g} + \mathcal{K}_2 Y_{2g}}{1 - Le(\mathcal{K}_1(\frac{11}{3} - Y_{1g}) + \mathcal{K}_2(-Y_{2g} - \frac{8}{3}))} \tag{5.90}$$

for the case of contiguous flame sheet and

$$\lambda = \frac{\mathcal{K}_1(Y_{1g} + \frac{11}{4}Y_{2g})}{1 + \mathcal{K}_1 Le(\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g})} \tag{5.91}$$

for the case of separated flame sheet.
From (5.89) and (5.91) it is straightforward to obtain the following criterion for the flame to be separated:

$$\mathcal{K}_1 > \frac{1}{Le}\frac{Y_{2g}}{\frac{8}{3}Y_{1g} + \frac{11}{3}Y_{2g}} \tag{5.92}$$

Notice that if $\mathcal{K}_2 \gg \mathcal{K}_1$ and $\mathcal{K}_2 \gg 1$ then

$$\lambda \sim \frac{1}{Le}\frac{Y_{2g}}{Y_{2g} + \frac{8}{3}} \tag{5.93}$$

for contiguous flame sheet. Similarly, in the case of separated flame sheet, if $\mathcal{K}_1 \gg 1$ we get the approximation

$$\lambda \sim \frac{1}{Le}\frac{Y_{1g} + \frac{11}{4}Y_{2g}}{\frac{11}{3} + Y_{1g} + \frac{11}{4}Y_{2g}} \tag{5.94}$$

5.5 Numerical solution

In this section we describe the numerical method employed to solve the equations given in section 5.3 defining the combustion of coal particles. This system have three unknowns, λ, δ_p and T_p. In a compact manner it can be written as follows:

$$\begin{aligned} \lambda &= G(\lambda, \delta_p, T_p) && (5.95)\\ \frac{d\delta_p^2}{dt} &= f(\lambda) && (5.96)\\ \frac{dT_p}{dt} &= g(\lambda, \delta_p, T_p) && (5.97) \end{aligned}$$

where G, f and g are defined in sections 5.5 and 5.6.
This system consists of one algebraic equation and two ordinary differential equations. To solve it we use the following discretization method:

Associated with a time step Δt we define approximations

$$\begin{aligned} \lambda^n &\simeq \lambda(t_n) \\ \delta_p^n &\simeq \delta_p(t_n) \\ T_p^n &\simeq T_p(t_n) \end{aligned} \tag{5.98}$$

where $t_n = n\Delta t$.
At step n we know λ^n, δ_p^n and T_p^n then we compute approximated values at time t_{n+1} by

$$\frac{\left(\delta_p^{n+1}\right)^2 - \left(\delta_p^n\right)^2}{\Delta t} = f(\lambda^n) \tag{5.99}$$

$$\frac{T_p^{n+1} - T_p^n}{\Delta t} = g(\lambda^n, \delta_p^{n+1}, T_p^{n+1}) \tag{5.100}$$

$$\lambda^{n+1} = G(\lambda^{n+1}, \delta_p^{n+1}, T_p^{n+1}) \tag{5.101}$$

Implicit equations (5.100) and (5.101) are solved by using Newton's method. We present numerical results to compare the solution of the model given in section 5.1 to the one corresponding to the asymptotic model obtained in section 5.4.
They have been computed for the following data taken from Libby and Blake [3]:

- ambient gas:

  $\rho_g = 0.241633$ kg/m^3, $v_g = 15$ m/s,
  $T_g = 1500,$ K $Y_{1g} = 0.11,$
  $Y_{2g} = 0.13,$ $Y_{3g} = 0,$
  $k = 6.61276\ 10^{-2}$ j/(mKs), $c = 1.1704\ 10^3$ j/(KgK).

- particles:

  $\rho_p = 1.5\ 10^3$ kg/m^3, $c_p = 2.006\ 10^3$ j/(KgK),

- chemical reactions:

  $B_1 = 1.1\ 10^4$ m/s, $E_1 = 1.75156\ 10^8$ j/mol,
  $B_2 = 3.8\ 10^5$ m/s, $E_2 = 1.49706\ 10^8$ j/mol,
  $q_1 = -1.43583\ 10^7$ j/Kg,
  $q_2 = 9.20157\ 10^6$ j/Kg,
  $q_3 = 1.0097\ 10^7$ j/Kg.

- radiation:

  $\epsilon = 0.9$, $\sigma = 5.6696\ 10^{-8}$ W/(m^{2}K^4), $I(\omega) = \frac{\sigma 1500^4}{\pi}$ W/(m^{2}str).

and the initial conditions

$$\delta_{p0} = 10^{-4}\ m, \qquad T_{p0} = 600\ K.$$

Figures 3, 4 and 5 show, respectively, the evolution in time of the radius of the particle, its temperature and the nondimensional combustion rate λ, obtained with both the "exact" and the "asymptotic" models.

Figure 3: Radius: ($*$) exact, ($\circ$) asymptotic

Figure 4: Temperature: ($*$) exact, ($\circ$) asymptotic

Figure 5: Nondimensional combustion rate: ($*$) exact, ($\circ$) asymptotic

6 Frozen gas-phase reaction

In the previous sections we have assumed that the gas-phase reaction (2.3) is infinitely fast. Now we address the situation where this gas-phase reaction is frozen.

6.1 A mathematical model

In this case the right-hand sides of the gas-phase equations (4.2)-(4.5) vanish because $w_3 = 0$ and hence we have

$$\rho v r^2 = \dot{m} \tag{6.1}$$

$$\frac{\dot{m}}{r^2}\frac{dY_1}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2\rho D\frac{dY_1}{dr}) = 0 \tag{6.2}$$

$$\frac{\dot{m}}{r^2}\frac{dY_2}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2\rho D\frac{dY_2}{dr}) = 0 \tag{6.3}$$

$$\frac{\dot{m}}{r^2}\frac{dY_3}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2\rho D\frac{dY_3}{dr}) = 0 \tag{6.4}$$

$$\frac{\dot{m}}{r^2}\frac{dT}{dr} - \frac{1}{r^2}\frac{d}{dr}(r^2\frac{k}{c}\frac{dT}{dr}) = 0 \tag{6.5}$$

and boundary conditions are

- At $r \to \infty$

$$Y_\alpha = Y_{\alpha g} \text{ for } \alpha = 1, 2, 3 \tag{6.6}$$

$$T = T_g \tag{6.7}$$

- At the surface of the particle: $r = \delta_p$

$$Y_\alpha = Y_{\alpha s}, \text{ for } \alpha = 1, 2, 3 \tag{6.8}$$

$$T = T_p \tag{6.9}$$

$$\dot{m}Y_1 - r^2\rho D\frac{dY_1}{dr}_{|r=\delta_p} = -\frac{11}{3}\dot{m}_1 \tag{6.10}$$

$$\dot{m}Y_2 - r^2\rho D\frac{dY_2}{dr}_{|r=\delta_p} = -\frac{4}{3}\dot{m}_2 \tag{6.11}$$

$$\dot{m}Y_3 - r^2\rho D\frac{dY_3}{dr}_{|r=\delta_p} = \frac{14}{3}\dot{m}_1 + \frac{7}{3}\dot{m}_2 \tag{6.12}$$

$$\dot{m}cT - r^2k\frac{dT}{dr}_{|r=\delta_p} = \dot{m}cT_p - \delta_p^2 q_g \tag{6.13}$$

After integrating two times we obtain

$$\begin{aligned}
Y_1 &= -\frac{11}{3}\frac{\dot{m}_1}{\dot{m}} + (\frac{11}{3}\frac{\dot{m}_1}{\dot{m}} + Y_{1g})e^{-\lambda\delta_p Le/r} && (6.14)\\
Y_2 &= -\frac{4}{3}\frac{\dot{m}_2}{\dot{m}} + (\frac{4}{3}\frac{\dot{m}_2}{\dot{m}} + Y_{2g})e^{-\lambda\delta_p Le/r} && (6.15)\\
Y_3 &= \frac{14}{3}\frac{\dot{m}_1}{\dot{m}} + \frac{7}{3}\frac{\dot{m}_2}{\dot{m}} + (-\frac{14}{3}\frac{\dot{m}_1}{\dot{m}} - \frac{7}{3}\frac{\dot{m}_2}{\dot{m}} + Y_{3g})e^{-\lambda\delta_p Le/r} && (6.16)\\
T &= T_p - \frac{\delta_p^2 q_g}{\dot{m}c} + \{T_g - T_p + \frac{\delta_p^2}{\dot{m}c}q_g\}e^{-\lambda\delta_p/r} && (6.17)
\end{aligned}$$

At the surface of the particle ($r = \delta_p$) we obtain the following values

$$\begin{aligned}
Y_{1s} &= -\frac{11}{3}\frac{\dot{m}_1}{\dot{m}} + (\frac{11}{3}\frac{\dot{m}_1}{\dot{m}} + Y_{1g})e^{-\lambda Le} && (6.18)\\
Y_{2s} &= -\frac{4}{3}\frac{\dot{m}_2}{\dot{m}} + (\frac{4}{3}\frac{\dot{m}_2}{\dot{m}} + Y_{2g})e^{-\lambda Le} && (6.19)\\
Y_{3s} &= \frac{14}{3}\frac{\dot{m}_1}{\dot{m}} + \frac{7}{3}\frac{\dot{m}_2}{\dot{m}} + (-\frac{14}{3}\frac{\dot{m}_1}{\dot{m}} - \frac{7}{3}\frac{\dot{m}_2}{\dot{m}} + Y_{3g})e^{-\lambda Le} && (6.20)\\
q_g &= \frac{k}{\delta_p}(T_g - T_p)\frac{\lambda}{e^\lambda - 1} && (6.21)
\end{aligned}$$

The two first of the above expressions are then used in (5.40), (5.41). Furthermore the heat flux to the gas phase is given by (5.39).
Finally, by introducing the nondimensional partial combustion rate numbers

$$\lambda_i = \frac{\dot{m}_i c}{k\delta_{p},} \qquad i = 1, 2 \tag{6.22}$$

we get the system of equations

$$\begin{aligned}
\delta_p\frac{d\delta_p}{dt} &= -\lambda\frac{k}{\rho_p c} && (6.23)\\
\lambda &= \lambda_1 + \lambda_2 && (6.24)\\
\lambda_1 &= \mathcal{K}_1\{-\frac{11}{3}\frac{\lambda_1}{\lambda} + (\frac{11}{3}\frac{\lambda_1}{\lambda} + Y_{1g})e^{-\lambda Le}\} && (6.25)\\
\lambda_2 &= \mathcal{K}_2\{-\frac{4}{3}\frac{\lambda_2}{\lambda} + (\frac{4}{3}\frac{\lambda_2}{\lambda} + Y_{2g})e^{-\lambda Le}\} && (6.26)\\
\frac{\delta_p}{3}\rho_p c_p\frac{dT_p}{dt} &= \frac{k}{\delta_p}(T_g - T_p)\frac{\lambda}{e^\lambda - 1}
\end{aligned}$$

$$\begin{aligned} &+ \quad \frac{k}{\delta_p c}(q_1\lambda_1 + q_2\lambda_2) \\ &+ \quad \epsilon(\frac{1}{4}\int_S I(\omega)dS(\omega) - \sigma T_p^4) \end{aligned} \tag{6.27}$$

where $\mathcal{K}_1$ and $\mathcal{K}_2$ are given by (5.45) and (5.73), respectively.

6.2 An asymptotic model

6.3 Numerical solution

In this section we show the numerical results obtained for the previous model. We have used the same numerical scheme as in section 5.5. Computations have been made for the data included there.

Figures 6 to 10 show, respectively, the evolution in time of the radius of the particle, its temperature and the nondimensional combustion rates λ_1, λ_2 and λ.

Figure 6: Radius

Figure 7: Temperature

Figure 8: Nondimensional combustion rate: reaction 1

References

[1] Burke, S.P. and Schumann, T.E.W. *Proc. Third Int. Bituminous Coal Conf.* 2, p.485. 1931.

[2] Libby, P. A. Ignition, combustion and extinction of carbon particles.*Combustion and Flame*, 38:285-300 (1980).

[3] Libby, P. A. and Blake, T.R. Theoretical study of burning carbon particles.*Combustion and Flame*, 36:139-169 (1979).

[4] Liñán, A. The asymptotic structure of counterflow diffusion flames for large activation energies. *Acta Astronautica*, 1:1007-1039 (1974).

[5] Liñán, A. Theory of droplet vaporization and combustion. In: *Modélisation des Phénomèmenes de Combustion*, R. Borghi, P. Clavin, A. Liñán, P. Pelcé and G.I. Sivashinsky, Eds. Eyrolles. Paris. 1985.

[6] Makino, A. An approximate explicit expression for the combustion rate of a small carbon particle. *Combustion and Flame*, 90:143-154 (1992).

[7] Makino, A. and Law, C.K. *Combustion Science and Technology*, 73:589-615 (1990).

Figure 9: Nondimensional combustion rate: reaction 2

[8] Matalon, M. Complete burning and extinction of a carbon particle in an oxidizing atmosphere. *Combustion Science and Technology*, 24:115-127 (1980).

[9] Matalon, M. Weak burning and gas-phase ignition about a carbon particle in an oxidizing atmosphere. *Combustion Science and Technology*, 25:43-48 (1981).

[10] Matalon, M The steady burning of a solid particle. *SIAM J. Appl. Math.* 42:787-803 (1982).

[11] Nusselt, W.Z. *Verh. Deutsch. Ing.* 68:124-128 (1924).

Figure 10: Nondimensional combustion rate: total