Single coal particle combustion

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Abstract

The study of single coal particle combustion provides an important insight into the general nature of solid combustion and allows us to better understand the combustion of pulverized coal. This report studied how the single coal particle combustion is influenced by several parameters. The influences of changing air temperature, wall temperature and particle size was examined, and the behaviours of particles from different coal types was evaluated. By using a one-film model implemented in Matlab, it was shown that an increase in both the wall and air temperature had similar effects on the coal particle - the combustion process was faster and the temperature of the coal particle increased. Bigger particles took longer to burn, and show lower maximum temperatures than smaller particles. The study of different coal types found that coal types with a high moisture content take a longer time to reach the same temperatures than coal types with less moisture.

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Contents

1. Introduction

The study of single coal particle combustion provides an important insight into the general nature of solid combustion and allows us to better understand the combustion of pulverized coal, used in pulverized coal plants [1]. During the combustion process of a single coal particle, a carbon char is produced after the moisture evaporates and the volatile component is released from the particle and burned (devolatilisation). The combustion of the coal particle then releases heat until all the carbon is burnt and only the non-combustible components of the particle, otherwise known as the ash, is left [1]. Figure 1 presents a simplified overview of the different steps of the combustion process.

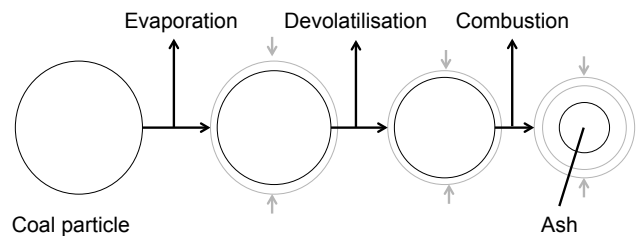For this report, the drop tube furnace was chosen as the model environment to study the single coal particle

Figure 1. Different steps of the combustion process

combustion process. The behaviour of the coal particle during the combustion process has important implications on the design of the furnace, where the particle is burnt, e.g. the necessary residence time, the volume, etc. [1]. Therefore, it is important to understand which factors, both coal-specific and environmental, influence the combustion process of the particle.
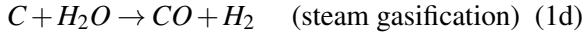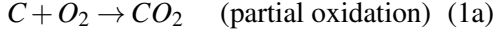
The report therefore studies the influence of the following factors:

- temperature of the air inside the furnace,

- temperature of the furnace wall,

- size of the particle, and

- type of coal.

The report is structured as follows: Section 2 introduces the model used to describe the combustion process, Section 3 presents and discusses the results of the model when changing the mentioned factors, and Section 4 concludes the report.

2. Methods

When a coal particle is released into the drop tube furnace, its surface gets attacked by either O_2, CO_2 or H_2O, mainly depending on the surface temperature [1]. The reactions on the surface of the coal particle are the following:

$$C + O_2 \rightarrow CO_2 \quad \text{(partial oxidation)} \quad \text{(1a)}$$
$$2C + O_2 \rightarrow 2CO \quad \text{(oxidation)} \quad \text{(1b)}$$
$$C + CO_2 \rightarrow 2CO \quad \text{(gasification)} \quad \text{(1c)}$$
$$C + H_2O \rightarrow CO + H_2 \quad \text{(steam gasification)} \quad \text{(1d)}$$

The main product on the particle's surface is CO, which then diffuses through the boundary layer and reacts with O_2 to become CO_2 [1]. This report ignored the production of CO and focused on Reaction 1a, since the production of CO is complex and is not necessary to get an overall understanding of the combustion process [1]. We therefore chose to adopt the so-called one-film model that makes the following assumptions:

1. The coal particle only consists of moisture[1], char, volatiles, and ash, and the change of the porosity of the coal particle when pyrolzing and burning is ignored [2]. Therefore, the density of the particle stays constant.

2. The coal particle is supposed to be spherical and burning in a quiescent, infinite, ambient medium that contains only oxygen and an inert gas, such as nitrogen [2]. There is no interaction with other particles, and the effects of convection are ignored. [1].

3. The flame is supposed to be infinitely thin, and spherically symmetric around the coal particle [2].

4. The pyrolyzing and burning process is quasi-steady [1, 2].

5. Only oxidation of coal char occurs at the particle surface producing CO_2 (Reaction 1a) [2].

6. The physical properties of coal and gas, such as the gas-phase thermal conductivity, specific heat, and particle density, are all constant at a certain surface temperature. Furthermore, the Lewis number is assumed to be unite, i.e., Le = 1 [1, 2].

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[1]The impact of moisture is examined later in the report.

7. The particle is of uniform temperature and radiates as a gray body to the surroundings without participation of the intervening medium [1].

8. Heat released during the combustion of the particle does not affect the air and wall temperature of the furnace.

Turns [1] used Figure 2 to illustrate the one-film model and the implications of its assumptions. The concentration of CO_2 is at its maximum at the surface of the particle and decreases with growing distance from the particle. In contrast to that, the concentration of O_2 is at its minimum on the surface, and converges to $Y_{O_2,\infty}$, the O_2 concentration of the environment.
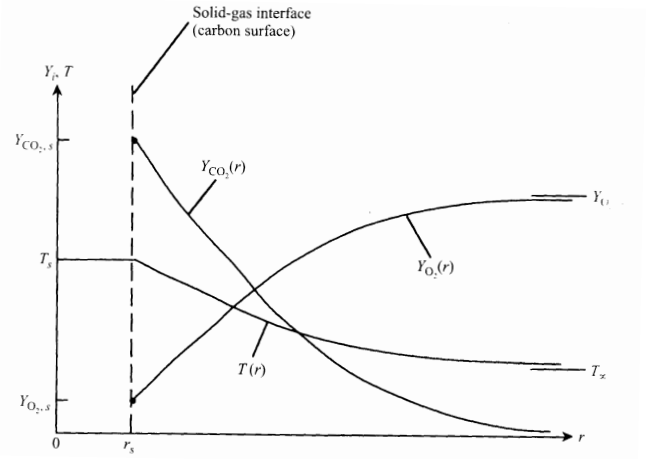

Figure 2. Species and temperature profiles of the one-film model

2.1 Formulas
This subsection introduces the formulas used to set up the one-film model.
Equations for constants
The initial mass of the spherical particle m_p was calculated by

$$m = \frac{\rho * \pi * d^3}{6} \quad (kg) \quad (2)$$

The initial mass of the volatile component V^* was calculated by

$$V^* = w_V * m \quad (kg)$$

The density of the air on the surface is dependent on the temperature of the particle T_p and was calculated by

$$\rho_{Air} = \frac{\rho_{abs} * MW_{Air}}{R * T_p} \quad \left(\frac{kg}{m^3}\right)$$

The mass diffusivity D was estimated using a value for CO_2 in N_2 and the temperature of the particle T_p [1] and was defined as

$$D = (\frac{T_p}{393})^{1.5} * 1.6e - 5 \quad (\frac{m^2}{s})$$

Equations for the one-film model

To describe the kinetics of the pyrolysis reaction (devolatilisation), we used a first order reaction for the total weight loss of the volatiles [3].

$$\frac{dV}{dt} = B_v * e^{\frac{-T_V}{T_p}} * (V^* - V) \tag{3}$$

The change of the particle's mass over time was derived from the burning rate of the carbon and the devolatilisation.

$$\frac{dm}{dt} = -\dot{m} - \frac{dV}{dt} \tag{4}$$

The change of the particle's diameter over time was dependent on the change of the particle's mass over time and its diameter.

$$\frac{dd}{dt} = \frac{dm}{dt} * \frac{2}{\pi * \rho * d^2} \tag{5}$$

The change of T_p over time was derived from the energy conservation throughout several energy- and mass-transfer processes [1]. These processes[2] were:

- combustion or chemical heat release,

- conduction with the surrounding air,

- radiation from the furnace walls, and

- energy loss due to the pyrolysis reaction.

To calculate the change of the T_p over time, the following equation was used:

$$\frac{dT}{dt} = \frac{1}{c_{p_p} * m} * [\dot{m} * \Delta h_C - \frac{dV}{dt} * \Delta h_V$$
$$- Nu * \lambda * \pi * d * (T_p - T_\infty)$$
$$- \varepsilon * \sigma * \pi * d^2 * (T_p^4 - T_{surr}^4)]$$
$$- \frac{T_p}{m} * \frac{dm}{dt} \tag{6}$$

In the implemented model, we assumed the Nusselt number Nu to be 2, therefore not taking into account convective effects. The emissivity of the particle surface ε was

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[2]The influence of the evaporation of moisture was considered in a separate model.

assumed to have the value of 0.8 [2]. The thermal conductivity was set to the value of 0.064 [7]. The energy released by burning the volatiles was not considered in this model.

The combustion rate of carbon at the surface of the particle is mainly influenced by two regimes, which are diffusionally and kinetically controlled.

Diffusionally controlled combustion occurs when the particle size is big and both the temperature and pressure are high. The combustion rate is controlled by the diffusion rate of oxygen to the particle's surface, at which its concentration , $Y_{O_2,s}$, approaches zero. In this regime, the combustion rate depends strongly on the boundary layer thickness and weakly on the chemical-kinetic parameters [1, 4]. The value of the Sherwood number Sh is assumed to be 2 for an isolated particle burning in a stagnant atmosphere [3].

$$\dot{m}_{diffusion} = (v_{1a})^{-1} * Sh * \pi * d * \rho_{air}$$
$$* D * (Y_{O_2,\infty} - Y_{O_2,s}) \tag{7}$$

Kinetically controlled combustion occurs when the particle size is small and both the temperature and pressure are low. In this regime, the diffusion of oxygen to the solid surface and the migration of gaseous products through the boundary layer into the freestream are much faster than the formation of products from adsorbed molecules on the surface [4].The combustion rate is then determined by chemical kinetics and therefore the process is kinetically controlled. The combustion rate on this regime exponentially depends on the surface temperature. Since the process of diffusion, being conducted through the boundary layer, is irrelevant in this regime, the combustion rate is independent of its thickness. Concentrations of oxygen at the reacting surface are not too different from those in the freestream [4].

$$\dot{m}_{kinetic} = v_{1a} * \pi * d^2 * \rho_{air} * Y_{O_2,s} * B_{1a} * e^{\frac{-T_c}{T_p}} \tag{8}$$

Both $\dot{m}_{diffusion}$ and $\dot{m}_{kinetic}$ are dependant on the oxygen concentration on the surface, $Y_{O_2,s}$. In order to calculate $\dot{m}$ and $Y_{O_2,s}$, we set both combustion rate equations equal to each other and solved for $Y_{O_2,s}$.

$$\dot{m}_{kinetic} = \dot{m}_{diffusion} \Leftrightarrow$$
$$Y_{O_2,s} = (\frac{v_{1a}^2 * d * B_{1a} * e^{\frac{-T_c}{T_p}}}{Sh * D} + 1)^{-1} * Y_{O_2,\infty} \tag{9}$$

Equations for one-film model with moisture

For an additional analysis, we included moisture in our one-film model. We assumed that as soon as the particle was released into the drop-tube furnace, the moisture would evaporate before the devolatilisation had started [9].

The change of mass of the moisture over time was modelled similar to the change of volatiles, however with a faster approach to the total mass of moisture.

$$\frac{dM}{dt} = 37e4 * e^{\frac{-4000}{T_p}} * (M^* - M) \tag{10}$$

When including moisture in the one-film model, we needed to adjust the formulas for the change of mass over time

$$\frac{dm}{dt} = -\dot{m} - \frac{dV}{dt} - \frac{dM}{dt} \tag{11}$$

and the change of temperature over time, since evaporation now influenced the temperature of the particle.

$$\frac{dT}{dt} = \frac{1}{c_{p_p} * m} * [\dot{m} * \Delta h_C - \frac{dV}{dt} * \Delta h_V$$
$$- Nu * \lambda * \pi * d * (T_p - T_\infty)$$
$$\Rightarrow \quad -\frac{dM}{dt} * \Delta h_M \tag{12}$$
$$-\varepsilon * \sigma * \pi * d^2 * (T_p^4 - T_{surr}^4)]$$
$$-\frac{T_p}{m} * \frac{dm}{dt}$$

Table 1 presents the values for the used parameters and indicates the source of the information.

2.2 Matlab implementation

The equations governing the particle mass and energy were implemented and numerically solved in Matlab [6]. For the initial value problem with the equations 3, 4, 5 and 6, the ode45 function was used. When the one-film model with moisture was used, the equations 3, 5 10, 11 and 12 were applied. The initial temperature of the particle was set to 300K, and the initial mass of the particle, diameter and volatile mass were calculated as described in Subsection 2.1.

With the help of the "events"-option in the ode45 function, the first computation was stopped as soon as only ash was left from the particle. At this point, combustion stopped since no combustible mass was left and the ash particle was only exposed to radiation from the furnace wall and conduction from the furnace air. This

Table 1. Table of Constants

Variable	Unit	Value	Source
c_{p_p}	$\frac{J}{kg*K}$	1286	[1]
ρ	$\frac{kg}{m^3}$	1350	[2]
Δh_C	$\frac{J}{kg}$	$32.80e6$	[2]
Δh_V	$\frac{J}{kg}$	$0.42e6$	[2]
Δh_M	$\frac{J}{kg}$	$2.40e6$	[5]
T_C	K	12148	[2]
T_V	K	8860	[2]
B_V	K	$37e4$	[2]
ε		0.8	[2]
B_{1a}	$\frac{m}{s}$	$1.2e4$	[2]
Sh		2	[3]
Nu		2	[6]
λ	$\frac{J}{m*K*s}$	0.064	[7]
ρ_{abs}	$\frac{kg}{m^3}$	101325	[1]
R	$\frac{J}{K*mol}$	8.314	[2]
σ	$\frac{m^2*kg}{s^2*K}$	$5.67e-8$	[2]
MW_{Air}	$\%$	0.03	[1]
$Y_{O_2,\infty}$	$\%$	23	[1]
v_{1a}		2.6636	[1]

process was then calculated in a second computation. When the temperature of the particle reached a stable point, hence radiation and conduction were in an equilibrium, the second computation was stopped.

3. Results and Discussion

This section presents and discusses the results from the combustion model introduced in Section 2. This is done by changing the model's parameters and evaluate the impact of the change on the behaviours of the

- mass of the particle,

- diameter of the particle,

- mass of the volatiles, and

- temperature of the particle.

Subsection 3.1 first evaluates the impact of a change in air temperature. Subsection 3.2 then concentrates on the change of the wall temperature. The impact of a changing particle size is evaluated in Subsection 3.3, by
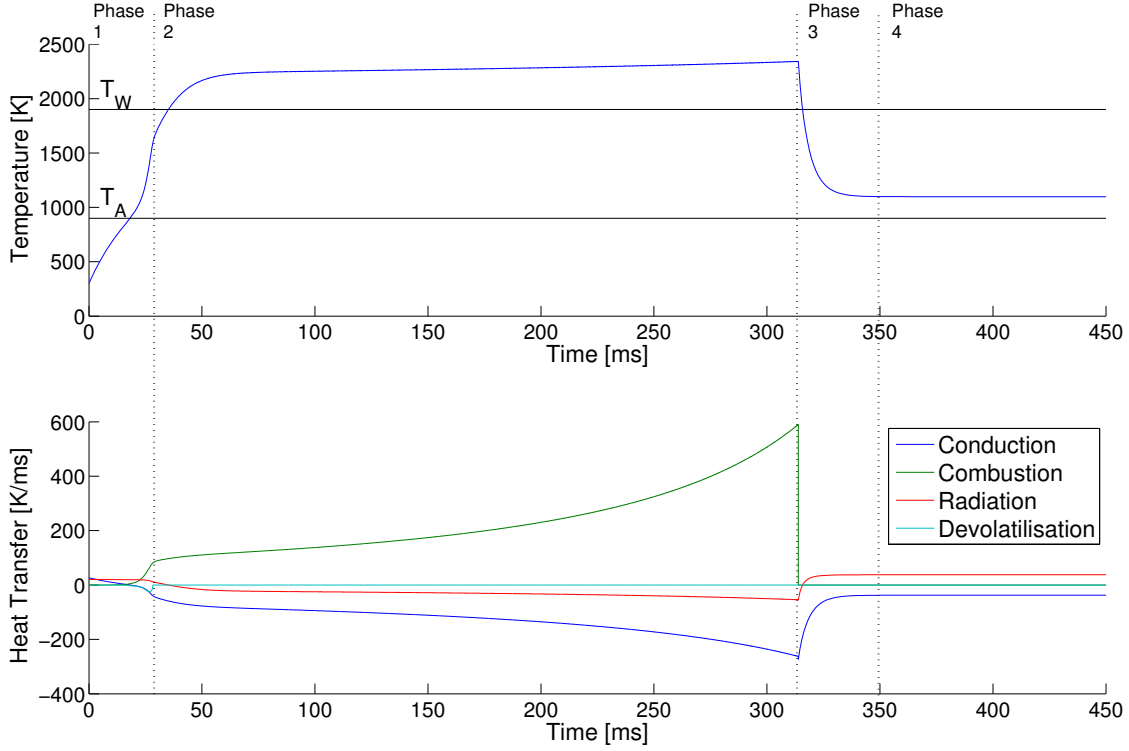
Figure 3. Heat Transfer and Temperature

changing the diameter of the particle. Finally, Subsection 3.4 examines the behaviour of different types of coal.

The first three analyses used a dry type of coal (w% Ash: 11.3, Volatiles: 32.5, Carbon 56.2, [2]) and ignored the impact of moisture. If not otherwise stated, the wall temperature was assumed to be 1800K, the air temperature was assumed to be 1200K and the particle size defined by the diameter was assumed to be $100\,\mu m$ [2].

In the absence of moisture, the combustion process of the particle can be divided into 4 phases:

1. devolatilisation & combustion,

2. combustion,

3. cooling, and

4. steady temperature.

Figure 3 presents the temperature of the particle over time, and the impact of the energy and heat processes during the residence time in the furnace. The chosen parameters were adequate to enable combustion of the particle. For the purpose of this graph, T_w was set to 1900K and T_a was set to 900K. This setting made it easier to distinguish the effects of the different heating and energy processes.

During *Phase 1*, the dominant processes were conduction, radiation, devolatilisation and a starting combustion. As soon as the particle was dropped into the drop-tube furnace, its temperature rose quickly since the temperature of the environment was much greater. Devolatilisation was initiated and reached its peak, just after the combustion started to play the dominant role in heating the particle. As soon as all the volatiles were detached from the particle, the devolatilisation stopped.

Phase 2 was mainly dominated by the combustion process. The burning rate of the particle increased with increasing temperature, resulting in a greater heat release through combustion. Since the temperature of the particle was now greater than both the wall and the air temperature, radiation and conduction had a negative impact on the particle's temperature, but were not strong enough to offset the heat release through combustion - hence, the temperature of the particle increased. The end of *Phase 2* marked the end of the combustion process, where all the combustible carbon was consumed and only ash was left from the particle.

Due to the absence of combustion, the coal particle cooled down in *Phase 3* and the temperature converged

to a steady-state where the impact of conduction and radiation was equal. The coal particle therefore did not change its temperature but remained between the temperature of the wall and the air (*Phase 4*). It is interesting to note that the temperature of the coal particle converged to a temperature closer to the air temperature.
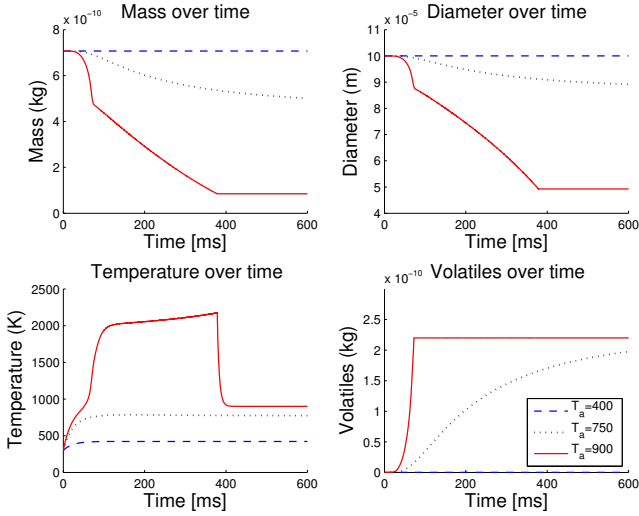

Figure 4. Particle behaviour from low to high air temperatures

Figure 4 shows the particle's behaviour when the air temperature was very low to fairly high. The wall temperature was set to 900K.

When the air temperature was very low (T_{air}=400K), neither combustion nor devolatilisation occured. The particle was only heated to the equilibrium temperature of radiation and conduction, the mass and diameter stayed constant since neither volatiles were released nor carbon was burned.

When we slightly increased the air temperature (T_{air} =750K), devolatilisation was possible, but still no combustion occured. The mass and diameter of the particle decreased since volatiles were released and the temperature converged to the equilibrium temperature of radiation and conduction.

If the environmental conditions (T_{air} =900K) were sufficient to enable devolatilisation and combustion, the temperature profile looked similar to the one shown in Figure 3. The 4 phases could be distinguished from the temperature graph. The mass and diameter profile looked similar since they were directly correlated (Equation 2). During *Phase 1*, the devolatilisation had the biggest impact on the size of the particle, since volatiles were removed from the particle, resulting in a smaller particle.

The burning rate of the carbon was low at the beginning, so the consumption of carbon had a low impact on the diameter and the mass. The impact of combustion on the diameter and mass was the biggest during *Phase 2*. Both the mass and the diameter decreased almost linearly, until only ash was left. The particle size remained constant for *Phase 3* and *Phase 4*.

3.1 Changing air temperature

This subsection evaluates the influence of different air temperatures on the behaviour of the coal particle during the combustion process. Three different air temperatures were used for this evaluation, at 800K, 1500K and 2200K.

Figure 5 presents the impact of changing air temperatures on the behaviour of the coal particle during the combustion process. It becomes evident that the combustion process took longer with decreasing air temperatures. In particular the duration of the devolatilisation was increased, since this process occurred at the beginning of the combustion process, when the particle was cold and the conduction from the air had a significant impact on the particle's temperature. The maximum temperature
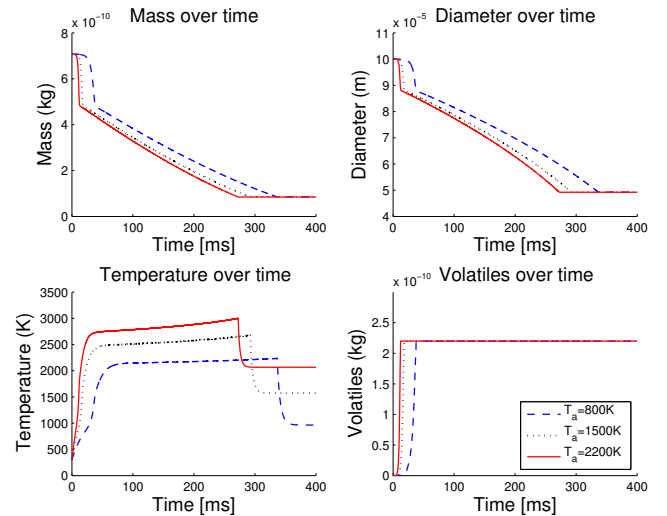

Figure 5. Particle behaviour for different air temperatures

of the coal particle during the whole combustion process also decreased with a decreasing air temperature, and the heat release from combustion towards the end of the combustion was mainly offset by radiation and conduction for colder air temperatures. This becomes evident when looking at the slope of the temperature curve - the slope was almost zero for the low temperature case.

Since we used the same coal type for each air temperature, the curves for mass, diameter and volatiles converged to the same limit. The different air temperatures only influenced the speed of this convergence.

3.2 Changing wall temperature

This subsection now evaluates the influence of different wall temperatures on the behaviour of the coal particle during the combustion process. Three different wall temperatures were used for this evaluation, at 800K, 1500K and 2200K.

Figure 6 presents the results for this analysis. Similar to the analysis of different air temperatures, the combustion process took longer with a decreasing wall temperature and the maximum and equilibrium temperature were lower.
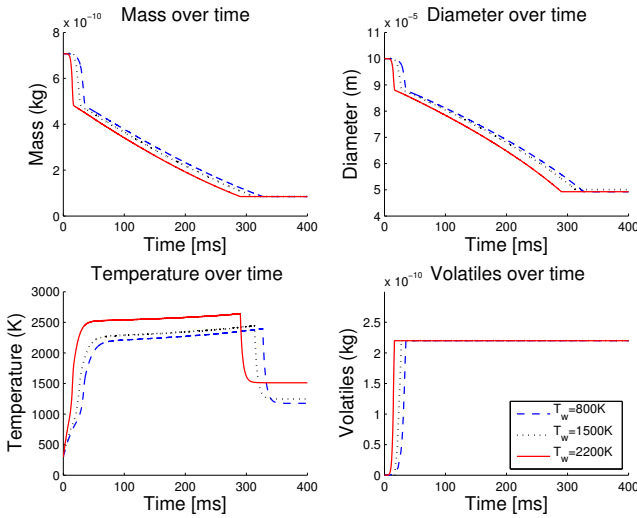

Figure 6. Particle behaviour for different wall temperatures

3.3 Changing diameter of particle

This subsection examines the influence of different particle sizes on the behaviour of the coal particle during the combustion process. For the purpose of this assessment, we changed the diameter of the particle, which directly translated into the mass (Equation 2). The diameters used for this evaluation were 50, 70 and 100 μm.

In Figure 7, it becomes evident that the combustion process took longer the bigger the particle was. It is interesting to note that whereas the time for *Phase 1* (devolatilisation) did not significantly change with a bigger particle, the time for *Phase 2* (combustion) did. In addition, the maximum temperature of the particle was

higher for smaller particles. The equilibrium temperature between radiation and conduction mainly depended on the wall and air temperatures and was not significantly influenced by the particle size.
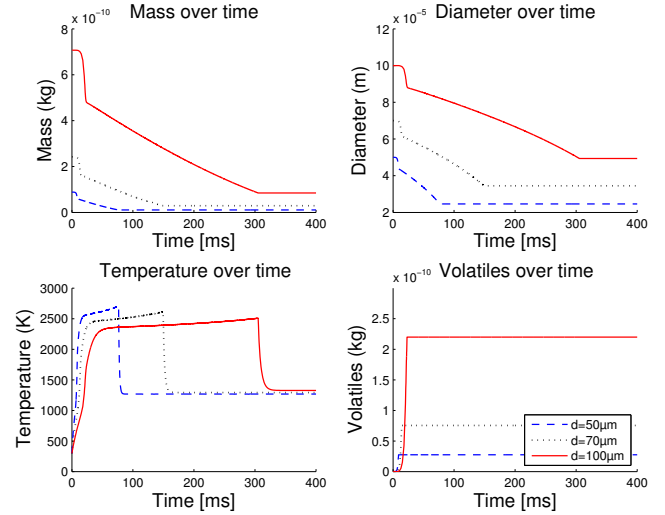

Figure 7. Particle behaviour for different particle sizes

3.4 Different types of coal

For the analysis of the impact of different types of coal on the behaviour of the particle, we used the coal types presented in Table 2. *Pittsburg* represented a coal with a high carbon content, *Hambach* a type of coal with a high volatile content, and *Fort Union* a type of coal with a lot of moisture. The dominant components of the coal types are marked in bold. In order to make an easy comparison of the behaviours possible, the density was assumed to be equal for all examined coal types.

Table 2. Coal types and their composition in w% [8]

Coal type	Carbon	Volatile	Ash	Moisture
Pittsburg	**56.2**	31.1	11.3	1.4
Hambach	37.5	**41.0**	3.5	18.0
Fort Union	30.3	26.3	6.2	**37.2**

In contrast to the previous subsections, we now included moisture in our analysis. We assumed that as soon as the particle was released, the moisture was evaporated before the devolatilisation had started [9]. Figure 8 adds the impact of evaporation to Figure 3. The pink area shows the heat transfer caused by the evaporation at the beginning of the residence time. Note

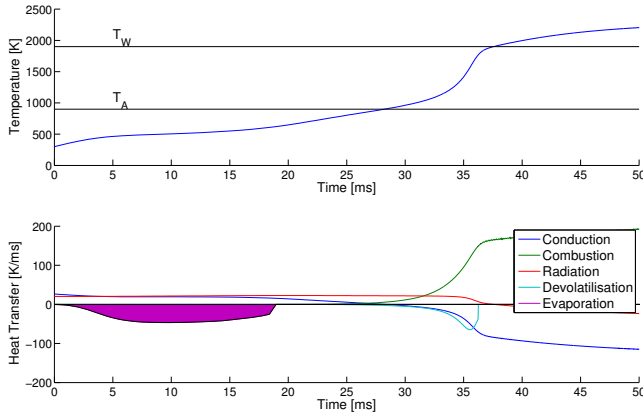that Figure 8 does not show the whole residence time, but zooms in when evaporation occurred.

Figure 8. Heat Transfer and Temperature with evaporation of moisture

Figure 9 presents the behaviour of the coal particle when different coal types were used. The graphs now show an additional phase, caused by the evaporation. This phase occurred before the devolatilisation. Since *Pittsburg* was the coal type with the lowest moisture component, the evaporation phase was small and its impact on the behaviour of the particle was negligible. Due to *Fort Union's* high moisture content, the evaporation phase was the longest and had the biggest impact on the mass, diameter and temperature of the particle. The mass and diameter dropped quickly since the moisture was evaporated. The necessary energy for this process resulted in a longer heating time required for *Fort Union* to reach the same temperature than the other two coal types.

Hambach was the type of coal with the highest volatile content, therefore the devolatilisation had the biggest impact on the particle's behaviour of all coal types. After a short period of evaporation, the mass and diameter dropped significantly for *Hambach* as the volatiles were released from the particle.

Phase 3 started for *Pittsburg* and *Hambach* around the same time, whereas *Fort Union* was delayed by around 10ms. This was mainly due to the time and energy it took to evaporate the moisture. *Fort Union* had the shortest *Phase 3*, since it was the coal with the lowest carbon content. *Pittsburg* had a shorter *Phase 3* than *Hambach*, even though its carbon content was bigger. This was related to the high ash content of *Pittsburg*, the highest among all coal types. Therefore, the mass and the diameter remained on the highest level af-

ter all the carbon was burned. *Hambach* had the smallest remaining particle.

Even though *Pittsburg* had the highest content of carbon, the maximum temperature was similar to *Hambach* and *Fort Union*. This was mainly caused by the high amount of ash in *Pittsburg* that resulted in a higher mass of particle to be heated, without an additional heat release.
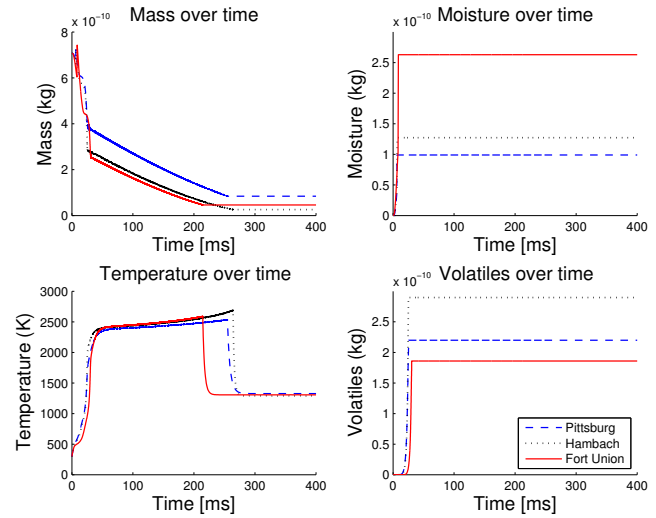

Figure 9. Particle behaviour for different coal types

4. Conclusion

The report studied the single coal particle combustion and how the combustion was influenced by several parameters. The influence of a changing air temperature, wall temperature and the size of particle was examined, and the behaviour of particles from different coal types was evaluated.

In general, if the environmental conditions were adequate to enable combustion, the behaviour of the coal particle could be divided in four, with moisture in five, phases: *evaporation of moisture*, devolatilisation and combustion, combustion, cooling and steady temperature.

By using a one-film model implemented in Matlab, it was shown that both an increasing wall and air temperature had similar effects on the coal particle: the combustion process was faster, and the temperature of the coal particle increased. Bigger particles took longer to burn, and had lower maximum temperatures than smaller particles.

The analysis of different types of coal took into account the impact of moisture and the required energy

to evaporate the water. It became evident that coal types with a high moisture content took a longer time to reach the same temperatures than coal types with less moisture.

Even though this study was able to evaluate how changing particle parameters can affect the combustion process, several limitations can be identified. First, the one-film model gives a good approximation to the combustion process, but does not take into account the production of CO. Second, the combustion of volatiles was neglected for this study, but can have an influence on the combustion process. Third, the heat conductivity was assumed to be constant, but is in fact dependant on the temperature of the environment.

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Nomenclature

d	diameter of particle (m)
m	mass of particle (kg)
V	mass of volatiles (kg)
V*	ultimate yield of volatiles at t = ∞ (kg)
M	mass of moisture (kg)
M*	ultimate yield of moisture at t = ∞ (kg)
ρ	density of particle ($\frac{kg}{m^3}$)
w	mass share (%)

Subscript

p	Particle
C	Carbon
V	Volatiles
A	Ash
M	Moisture

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