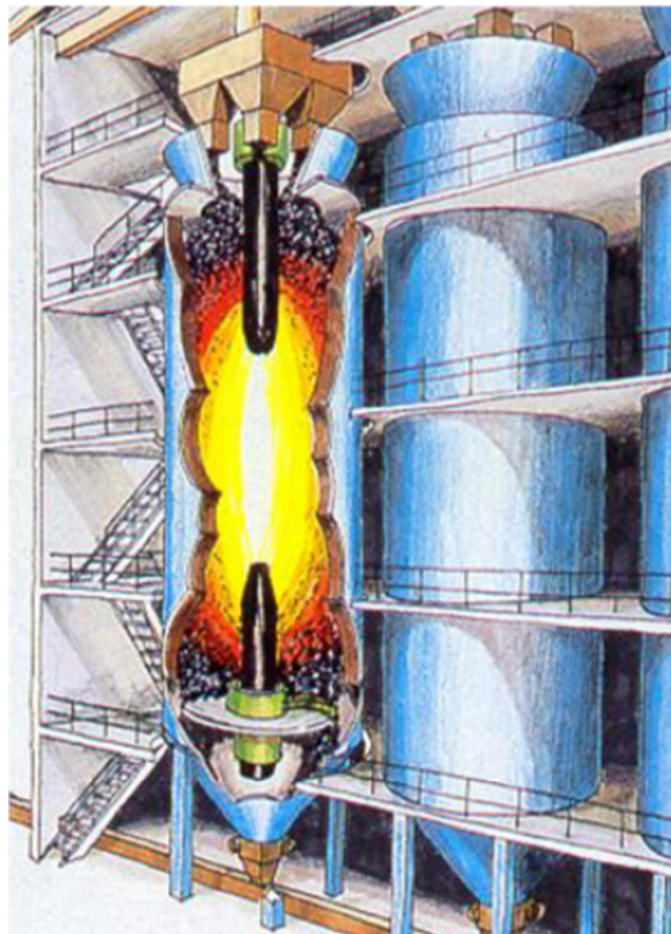


EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling



Thermal Electrical Behaviour of a Calciner

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1. Introduction

Background

The process of calcination involves the thermal treatment within a furnace of materials in order to facilitate various chemical transformations. This is applied in industry to obtain materials with properties that are tailored to some specific purpose. Possible applications include manufacture of electrodes and ramming pastes, which are used to fill seams in cathode blocks and furnaces. Therefore, an important objective is to produce a material that has low resistivity and can withstand extremely high temperatures and pressures. The furnace that we are concerned with is called a Calciner, as shown in Figure 1. The process involves the heat treatment of anthracite, a type of coal. The goal is to obtain a partly “graphitised” form of anthracite, that is, a material whose chemical properties resemble those of graphite. Graphite is an extremely desirable material in the metallurgy industry due to its superior ability to conduct electricity; however, manufacturing pure graphite is very expensive. However, by heating anthracite, a material can be obtained that exhibits similar characteristics to graphite for a much lower price. Anthracite is chosen due to its very high (92% - 98%) carbon content.

The Calciner is a cylindrical furnace that uses large alternating currents in the heat treatment of carbon.

The Calciner is a large cylindrical furnace, or what is described as a “shaft furnace”, and is approximately 8m in height and 2m in diameter. The furnace contains two electrodes, one at the top and one at the bottom, between which large alternating currents are applied. The anthracite is added continuously around the top electrode in granular form, and removed from the bottom via “scrapers”. It passes through the furnace due to gravity and hence experiences pressure from the particles above; its speed is determined by the rate of product removal by the scrapers. The particles conduct the electric current, and the resulting Joule heating drives the required graphitising transformation. The temperatures observed within the Calciner range from 1200°C to above 2500°C.

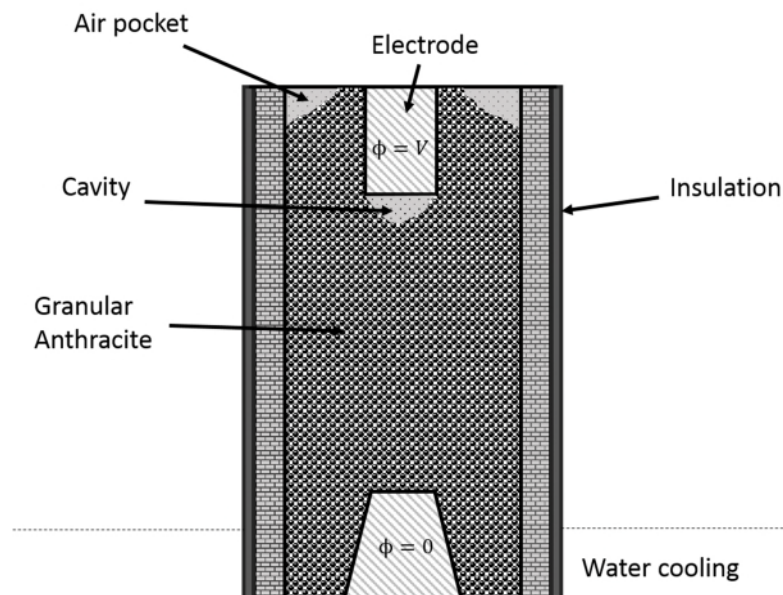


Figure 1: A schematic of a Calciner. The Calciner is a cylindrical furnace where anthracite particles are passed between two electrodes. The particles experience Joule heating as a consequence of the large alternating currents within the furnace.

Transformation of Anthracite during the Calcination Process

As the anthracite moves through the Calciner and is subject to high temperatures, it undergoes various transformations. Three critical processes are known to occur. The first of these is called **carbonisation**, which is the pyrolysis of anthracite due to the expulsion of volatiles. Impurities naturally occur within anthracite, particularly sulphur, hydrogen, nitrogen and oxygen, along with ash. It is important to drive off as high a proportion of these volatiles as possible, since we wish to obtain as pure a form of carbon as we can. Carbonisation takes place at the top of the furnace around the top electrode. Care must be taken when dealing with the by-products resulting from carbonisation. The resulting off-gas is generally burnt in order to combust the substantial quantities of hydrogen and carbon monoxide contained in it.

The second critical process is called **densification**, which describes the shrinkage of anthracite particles due to changes in its density. It is important that densification takes place within the Calciner, otherwise, when using the product to make electrodes, there is a risk of producing an electrode that will undergo structural changes and contract when in use. The threshold for such thermophysical stability is around 1200°C.

The third and final critical process is **graphitisation**. This is the irreversible mechanism that determines the partial transformation to graphite by means of changing the electrical resistivity of the anthracite. Heat treatment of coal causes its resistivity to decrease, however very high temperatures are required to reduce the resistivity to resemble that of graphite.

During the calcination process, the physical properties of anthracite are transformed to resemble those of graphite.

2. Properties of Anthracite

We consider the current conduction through a coke bed, and we discuss its bulk resistivity. With reference to Figure 2, we suppose that a coke bed comprises a collection of coke (anthracite) particles that are tightly packed and in contact with each other. The particles will experience a pressure or load as a consequence of the weight of the other particles in the coke bed.

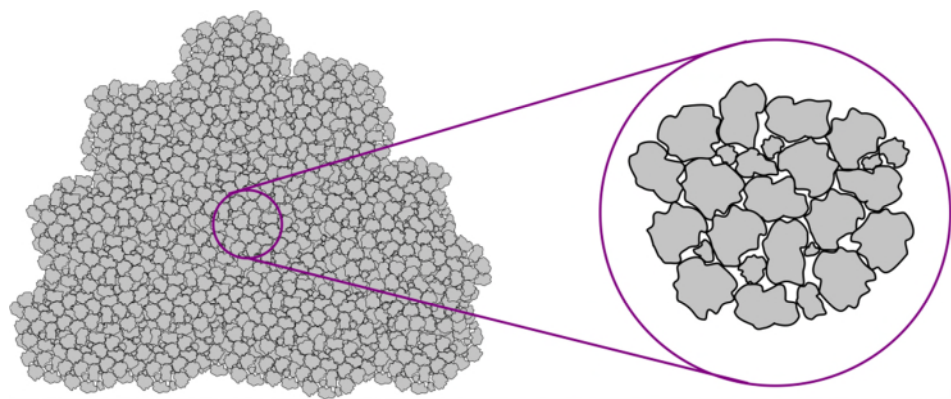


Figure 2: A coke bed is a collection of coke particles. The bulk resistivity of a coke bed is dependent on the material resistivity of the particles along with the resistance at the contacts between particles. Anthracite particles have rough surfaces, therefore have intricate and complex contact points.

The particulate behaviour of the anthracite is extremely important when understanding the bulk resistivity of a coke bed, not to mention how the material moves through the furnace. The bulk resistivity describes the total resistivity of the coke bed which we expect to be determined by the material resistivity and the resistance at the particle-to-particle contact points.

Resistivity

As mentioned, the anthracite in a Calciner is exposed to extremely large temperatures due to Joule heating as a consequence of the high currents. The resistivity, along with other physical properties, is temperature-dependant. Therefore the material resistivity of calcined anthracite differs depending on what temperatures the particles have experienced. Experimental results imply that material resistivity decreases with temperature. This is observed in experiments conducted by Elkem, as displayed in Figure 3.

The bulk resistivity of a bed of anthracite particles decreases with an increase in temperature. It is also observed that beds of larger particles have lower resistivity than those of smaller particles.

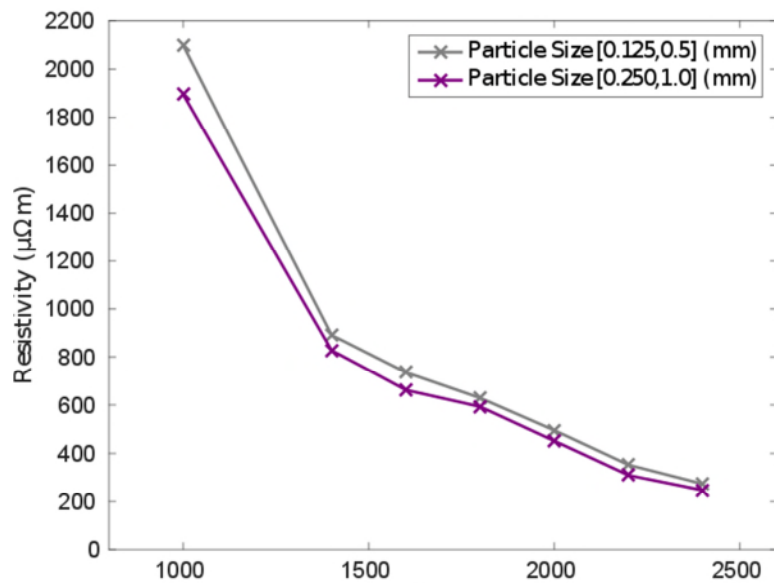


Figure 3: We see how the bulk resistivity of beds of anthracite particles of different size fractions depends on temperature. The general trend is that resistivity decreases with an increase in temperature.

Overall, we expect the bulk resistivity to depend on the resistivity of the material and the contact resistance where particles touch. The two samples being considered in Figure 3 consist of particles of different size ranges, namely 0.125-0.5mm and 0.25-1mm. At each of the temperature values, the resistivity of the smaller particles is greater than that of the larger particles, which implies that resistivity decreases with an increase in particle size. This effect has been explained in the literature, linking an increase in particle size to an increase in porosity. Porosity is directly linked to the strength of a particle, and hence when particles come into contact under pressure, the strength of the particle will play an important role in determining the contact area between particles, and consequently the contact resistance.

The surface structure of anthracite plays an important role in determining the contact areas between particles and hence the contact resistance.

Surface Structure

Electrical contact resistance is primarily governed by the surface structure and applied load. These two contributors are closely related, since forces upon contacting particles will cause deformations of the particle structure, in particular the structure of the surfaces in contact. Such deformations are likely to increase the contacting area, allowing for increased current conduction and hence a reduction in contact resistance. It is believed that larger particles are more likely to exhibit such deformations and exhibit greater contact areas and therefore experience less contact resistance.

Anthracite particles are quite angular in shape, with rough surfaces consisting of many corners and edges. When two such particles come into contact, their apparent contact area is much greater than the true contact area. Due to the complex and jagged structure of their surfaces, anthracite particles come into contact at only a collection of small regions. This restricts the current flow and hence we experience a build-up in current density at the regions of contact, resulting in a high resistance at the contact point.

3. Problem Definition

Modelling Electrostatics Problems

We are interested in understanding how current conducts through the packed bed of anthracite particles, and therefore we need to understand the theory of electrostatics. The physical quantities involved are the:

- **Current density \mathbf{j}** , which describes charges in motion and is defined as the electric current per unit cross-sectional area.
- **Electric field \mathbf{E}** at a given point, which is the force that would be exerted on a unit charge.
- **Electric potential φ** , which is the amount of electric potential energy that a unit charge would have at any point in space.

In order to understand how current is conducted through the anthracite particles, we must understand how the current density, the electric field, and the electric potential interact. We also need to obtain some quantification of how the conductivity of the material varies spatially within the furnace. The conductivity is the reciprocal of the resistivity, i.e. conductivity = (resistivity)⁻¹. The equations that govern our system are

$$\mathbf{E} = -\nabla\varphi, \quad \mathbf{j} = \sigma\mathbf{E}, \quad \nabla \cdot \mathbf{j} = 0, \quad (1)$$

where $\sigma(\mathbf{x})$ denotes the conductivity, which depends on the spatial coordinate \mathbf{x} . The second equation is Ohm's Law which relates the current density to the conductivity and the electric field. By combining these equations, we obtain an equation for **steady current conduction within solid anthracite particles**:

$$\nabla \cdot (\sigma \nabla\varphi) = 0. \quad (2)$$

As well as conductivity σ varying throughout the coke bed depending on the particle position, the inclusion of contact resistance between the particles will also impact the bulk conductivity. We therefore understand the conductivity to be a complicated function that varies rapidly on the microscopic scale, i.e. on the scale characterised by the length of a particle.

Within the coke bed, we assume any space not occupied by anthracite to be occupied by air, and we enforce zero conductivity in these spaces. Therefore, we must enforce a boundary condition for the electric potential at the interface between anthracite and air:

$$(\nabla\varphi) \cdot \mathbf{n} = 0, \quad (3)$$

where \mathbf{n} is the unit normal to the boundary. This equation describes the condition that there is no current flow across such a boundary.

Modelling the Coke Bed

Given the complicated surface of anthracite, we need to model the contact between particles carefully in a bid to capture this reduced area for current to flow. This problem is often tackled by approximating the surfaces as a set of asperities. The asperities themselves are modelled as some conjectural shape, for example spheres or ellipsoids. The heights of such asperities are statistically distributed.

As an alternative to asperity modelling, fractal theory has been applied in order to understand the true contact area between rough surfaces. The concept of a fractal is described as the middle-ground between linear geometric order, as observed in classical geometry and calculus, and geometric chaos, as observed in nature. Fractals are described as self-similar shapes, whose roughness neither vanishes nor fluctuates up and down when one continuously zooms in

To begin with the simplest case, we study the contact between identical, non-overlapping, smooth, elastic spheres. This study will lead to the natural extension of considering asperities upon our smooth surfaces, resulting in a fraction of the apparent contact area to be disregarded.

Allow the spheres to have radius r and to be arranged on a cubic lattice, where their centres are a distance L apart, as in Figure 4(a). Each sphere is in contact with six other spheres, therefore has six contact points. Pressure on the spheres which causes them to compress at their contact points, resulting in a circular contact area at each point.

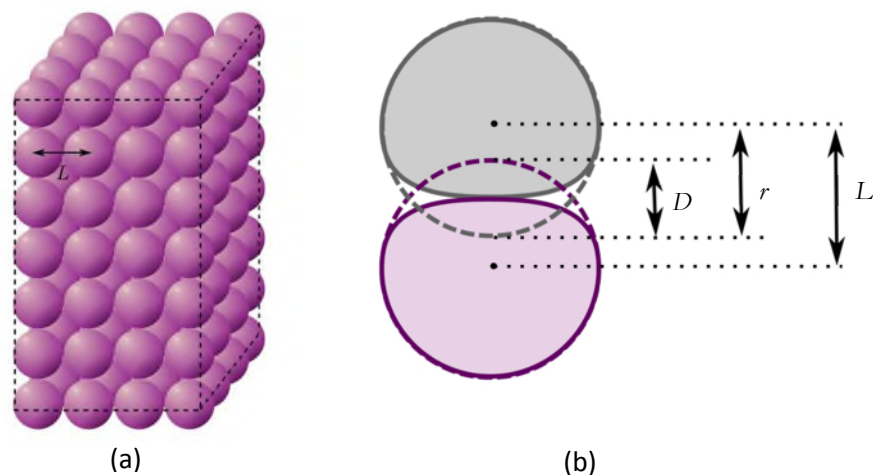



Figure 4: We visualise the coke bed in (a). The spherical particles are identical and placed on a cubic lattice, where L is the distance between their centres. They experience some pressure that forces them to compress. This compression is represented in (b) where we observe this phenomenon in two dimensions. The spheres have radius r and are compressed a total depth D .



Using results of Hertzian contact theory, we deduce that **the radius of the contact area** between two spheres in Figure 4(a) is

$$a = \sqrt{r \left(r - \frac{L}{2} \right)}.$$

This defines the area through which current can conduct. As mentioned before, this is for smooth spheres. The inclusion of asperities on the particle's surface will result in a decrease in this area.

Homogenisation

We have defined a system governed by equations (2) & (3). However, given the complex conductivity function σ , these equations are very difficult to solve. The conductivity varies on the length scale of a particle, however, when considering the geometry from the perspective of the entire furnace, these variations occur extremely rapidly. We are therefore interested in replacing this function with an **effective conductivity** that allows us to reduce the complexity of the problem while retaining the important characteristics.

The technique we apply is known as **the method of multiple scales**, and involves the definition of a macroscopic and microscopic length scale. We assume that this micro-scale problem will be the same regardless of its position within the furnace. This allows us to analyse the problem on the micro-scale to obtain an effective conductivity function which we can then apply to solve the macro-scale problem.

Homogenisation techniques allow us to reduce the complexity of the problem by obtaining an effective conductivity function.

4. Discussion, Conclusions and Recommendations

Through the implementation of the techniques and methods described in this document, we aim to understand the steady current conduction through a bed of anthracite particles within the Calciner. It is of greatest interest to understand how the particle material resistivity changes with temperature and the surface structure of the particles. The contact resistance between particles contributes to the majority of the bulk resistivity of a coke bed, therefore it is important to consider the interfaces of contact between particles.

In order to derive a mathematical model describing the behaviour of the electric current within the bulk material, it is vital to understand the intricacies of the contact points between particles, and how the current behaves when it is forced to converge through such a small interface. It would be beneficial for Teknova to explore the interactions between particles, in particular, in order to determine at how many points we expect a particle to make contact with surrounding particles. The collection and analysis of experimental data would be valuable to support and validate the mathematics, and will allow greater intuition and insight into the physical behaviour of this complex and detailed process.

Potential Impact

Svenn Anton Halvorsen, Chief Scientist at Teknova, commented *“This is an interesting work on understanding conductivity in particle beds. It will supply valuable support to a major on-going project: ‘Electrical Conditions in Metal Processes’, EIMet. The methodology can supply valuable, novel insight into conditions close to the tip of the electrodes in metallurgical furnaces. Such knowledge can potentially lead to large improvements in design and operation of the processes.”*