MODELLING
UNDERGROUND COAL GASIFICATION
MODELLING
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ONDERGRONDSE KOLENVERGASSING

PROEFSCHRIFT

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Chapter 1

Introduction

Underground coal gasification is a potentially attractive method for recovering the huge coal resources that cannot be mined using conventional methods. The objective of this study is to develop an integrated mathematical model of the cavity gasification process. Dedicated experiments are performed to assist model development.

1.1 Future Energy Demands

Over the past century world oil production showed a continuous increase, except during the politically induced energy crises of 1973 and 1979. It is expected that this increase will come to an end somewhere in the beginning of the twenty-first century [1]. After that, projected oil production will decrease in spite of technological developments and discoveries of new oilfields. This implies that in the future, countries with declining oil and gas reserves will become increasingly dependent on oil imported from countries and regions with more abundant reserves, such as the Middle-East and Venezuela.

In view of the close correlation between oil consumption and the growth of the world's population [2], it is of crucial importance that measures are taken to meet the expected future energy demands.

Coal is by far the most abundant alternative fossil energy source, with a proven economically recoverable reserve at end 1994 [3], of 782 billion ‘tonnes of coal equivalent' worldwide. This economic reserve represents 235 years of coal consumption at the 1994 level of production. The total coal resources, including currently economically unrecoverable coal deposits (also referred to as “greenfield coals") are estimated at more than 6700 billion tonnes of coal equivalent [4].

These vast amounts of coal represent an enormous potential energy source which could be used to fill the future gap between energy consumption and oil production. A prerequisite for filling this gap is that techniques are developed to recover currently unrecoverable coal resources. Underground coal gasification is

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1A ‘tonne of coal equivalent' is equivalent to a tonne of coal with a calorific value of 7000 [kcal/kg].
one of the methods that can possibly be applied to recover the greenfield coals in the world.

Underground coal gasification is of particular interest to the Netherlands. The Netherlands possesses considerable amounts of coal (estimates range from a few billion tonnes to tens of billion tonnes of greenfield coal [5, 6]) which are deep-seated and limited in thickness. The dependency of the Netherlands on their own steadily depleting natural gas resources and the political decision to postpone the development of nuclear energy make it all the more necessary to search for alternative domestic energy sources.

1.2 Underground coal gasification

The concept of underground coal gasification is simple: instead of recovering the coal itself, the coal is converted into combustible gas in situ by means of injecting air into the coal layer which partially oxidizes the coal. The gas thus produced is recovered via a vertical production well, and can be utilized for electricity generation, or converted to other usable products [7], see also Fig. 1.1.

The concept of underground coal gasification was proposed as early as 1873 by Sir William Siemens [8]. In the former Soviet Union, large-scale projects were carried out in shallow thick coal layers in the 1950s [9]. In Europe, various field trials were carried out in Belgium, Czechoslovakia, France, Germany, Italy, Poland, and the United Kingdom in the period 1940-1960 [10], with varying degrees of success.

During and after the oil crisis of 1973, there was considerable interest in alternative energy sources such as underground coal gasification. In the United States, several field trials were performed in thick and shallow or steeply dipping coal layers [11–14]. Results of these field trials showed that the underground gasification process was competitive with standard (aboveground) coal gasification techniques [11], at the then current energy and installation prices. The low energy prices of today, however, preclude commercial development of underground coal gasification in favourable coal deposits.

Deep-lying, thin coal seams such as exist in North-Western Europe can possibly be recovered economically by applying standard directional drilling techniques. Underground coal gasification is getting renewed interest in both Western and Eastern Europe because of the huge amounts of coal that are otherwise unminable in the European continent. A field test is currently being carried out in Spain, sponsored by the European Union. Former East-Bloc countries are also showing interest in this method of exploitation of coal resources.
1.3  CAVITY OR CHANNEL GASIFICATION METHOD

For horizontal or slightly dipping coal layers the cavity or channel gasification method is widely accepted to be the most efficient way of gasifying coals in situ. In vertical or steeply dipping coal layers a similar method is usually adopted, in which the gasified region is allowed to collapse to minimize the gasification cavity in size.

A typical well configuration for cavity gasification consists of a horizontal injection well with a vertical production well (see Fig. 1.1). Prior to gasification, a linkage path is created between injector and production well. The gasification step starts by igniting the coal and injecting air or air enriched with oxygen from the tip of a horizontal well, at the bottom of the coal seam. Subsequently, a cavity begins to form in the coal seam. Permeable bed gasification dominates the initial stages of cavity development. In the later stages, cavity surface gasification becomes more important. When the gas quality deteriorates the injection well is moved further upstream [16]. This technique is called controlled retraction of injection point (CRIP). Figure 1.2 depicts a conceptual picture of such a CRIP process. Several underground coal gasification field tests were designed for two or more CRIP steps [11,12,14]. For the process to be economic in thin coal layers, a cavity must develop of which the areal extent is much larger than the layer.
thickness. This is the main challenge for underground gasification of thin coal layers.

Several simulation models have been developed that describe the growth of a gasification cavity in coal seams [17–20]. All these models describe the evolution of an existing cavity. Most of these models only describe the expansion of the cavity as a result of chemical reactions and disregard mechanical failure mechanisms, or vice versa.

Van Batenburg [21, 22] has developed a model that includes both chemical reactions and roof failure. Its purpose, however, was to show that acceptable gas compositions could be attained by cavity gasification. It does not predict the areal sweep efficiency. His modelling results were confirmed by Kuyper [23], who developed a theoretical model which can describe the reactive natural convection flows and related transport phenomena in developed underground coal gasification channels, again with no limit for the areal sweep.

The transition from the early stages of gasification to a fully developed gasifier is still poorly understood. Key processes that influence this transition are: permeable-bed gasification, coal-surface gasification and roof-failure mechanisms. Important parameters are the ash content of the coal, permeabilities (of ash, roof debris, and char), coal- and roof-failure rates, well outlay and injection strategy. Development of a cavity is the result of an interplay between all these factors. From the early stages of gasification to a fully developed gasifier, natural convection flows play an increasingly important role.

As the influence of natural convection is the least well understood, part of this thesis is dedicated to fundamental aspects of natural convection under the prevailing conditions of underground coal gasification. Modelling cavity development, from the initial stages to a fully developed gasifier, is the subject of this
thesis.

1.4 Objectives and approach

The objective of this study is to develop an integrated mathematical model that can predict the development of a gasifier from the initial stages to a fully developed, mature cavity.

The model should comprise the following mechanisms: flow of gases through porous media, natural convection, chemical reactions, and coal- and roof-failure mechanisms. The roof-failure mechanisms are studied in detail elsewhere [24]. Here the emphasis is on reactive natural convection flows, and we combine these new observations with results from previous studies [22,23,25] and field trials [26–30].

To obtain input data for the model we have carried out a series of dedicated experiments, notably on natural convection flows and reaction mechanisms. Kuyper [31], developed a theoretical model of double diffusive, i.e., temperature- and composition-driven natural convection flows, but the model was never validated experimentally. We have constructed two experimental set-ups in which a comparison is made with the turbulence models that Kuyper used for his overall coal gasification model. In the set-ups, the (average) flow velocities and turbulence intensities are measured by means of a laser Doppler anemometer. From the validated simulations, local mass transfer coefficients can be extracted which in turn can be used in our integrated model.

Scaled high-pressure and -temperature gasification experiments are performed in this study to investigate the process under controlled laboratory conditions. During the experiments, gas composition and temperature can be monitored online at several locations. Experimental results provide us with indications for the minimum temperatures that are needed to sustain the reaction mechanisms which render the gasification process successful.

The model that is developed here can assist in interpreting the results of the field test, sponsored by the European Union, which is currently being conducted in Spain. It can also be used to extrapolate results from previous field trials in thick, shallow coal layers to North-Western European conditions, where coal layers are thinner, and located much deeper.

1.5 Thesis outline

In addition to the introduction, this thesis consists of five self-contained chapters, which are all dedicated to quantify or show the significance of natural convection for underground coal gasification modelling. Chapter 2 presents a three-dimensional model for the development of an underground coal gasifier. The
physical model combines both permeable-bed and cavity-surface gasification with thermo-mechanical failure of both coal and overlying rock. From the physical model, we turn to the numerical model with which some example calculations are carried out, in order to identify the important process parameters.

Chapters 3 and 4 describe experiments regarding natural convection flows. In Chapter 3, temperature-driven natural convection flows are studied, while Chapter 4 describes double-diffusive natural convection flows. Each of the chapters gives a description of the experimental set-up in which the laser Doppler velocity measurements take place.

In Chapter 3, temperature-driven natural convection flows are studied in a rectangular, differentially heated enclosed cavity, which is placed under different angles.

Chapter 4 studies double-diffusive natural convection flows, i.e., flows driven by both temperature and composition differences, in a trapezoidal configuration.

In both chapter 3 and 4, experimental results are compared with results from the numerical models developed by Kuyper [23]. The validated numerical modelling results provide us with estimates for the local mass-transfer coefficients that can be used as input for the integrated model presented in Chapter 2.

In Chapter 5, we describe high-pressure coal-gasification experiments, and discuss the results obtained from these experiments. Again, a comparison is made with results obtained from numerical models [23].

Finally, Chapter 6 uses the model presented in Chapter 2 for interpreting the results of the field tests.

1.6 Units and symbols

The units used in this study conform to the SI Metric System of Units, the notation is the one recommended by the Society of Petroleum Engineers. Each chapter ends with a list of symbols and their units.
Bibliography


BIBLIOGRAPHY


Chapter 2

An Integrated Model for UCG

In this chapter we develop and present a three-dimensional model for underground coal gasification. Essential features of the gasification process such as cavity gasification, permeable-bed gasification, and thermo-mechanically driven coal and roof failure have been integrated into a single model. Example calculations show that, for a representative combination of input parameters, a fairly high sweep efficiency is reached before breakthrough.

2.1 Introduction

Deep-lying, thin coal seams such as exist in North-Western Europe can possibly be recovered economically by the application of underground coal gasification in combination with standard directional and horizontal drilling techniques. A typical well configuration consists of a horizontal injection well and a vertical production well such as described in Chapter 1. In this configuration, the controlled retraction of injection point (CRIP) enables renewed gasification when the quality of produced gas deteriorates. A typical CRIP-step length can range from 5 to 20 metres, depending on the coal layer thickness.

The design of an underground coal gasification field test and its interpretation would greatly benefit from a dedicated simulator. In the past, many simulation models have been developed to describe gasification cavity development [1-5]. All these models are based on the assumption that a cavity already exists in the coal layer, and disregard one or more important aspects of the gasification process. We are the first to develop a model which describes cavity growth from the beginning, combining both chemically and mechanically driven cavity growth.

Here we present a 3D model that can be used to: (1) describe the transition from the early stages to a fully developed gasifier, and (2) predict the areal sweep efficiency. The model captures the essential features of the underground gasification process. It addresses the influence of ash permeability on overall cavity development, as well as the thermo-mechanically induced spalling of both roof rock and coal.
Figure 2.1: A 3D schematic representation of a coal layer with overlying roof rock (dashed lines), including well layout during the first CRIP step. It should be noted that injection takes place from the tip of a horizontally drilled well.

The model includes aspects of permeable-bed gasification, natural convection-driven cavity-surface gasification and roof-failure mechanisms. The model calculates the form and shape of the cavity. Long-term development of the cavity is dominated by natural convection-driven cavity gasification.

The main applications of the 3D model are the design and evaluation of underground coal gasification field trials, as well as extrapolating field-test results to the deep-lying thin coal seams such as exist in North-Western Europe. Finally, the model can be used to pinpoint important process and operating parameters.

2.2 Physical Model

2.2.1 Structural configuration

Consider a horizontal coal layer with a thickness $h$, length $L$, and width $W$, with a rock layer on top of it. A 3D representation is shown in Fig. 2.1, and a vertical cross-section at $W/2$ is shown in Fig. 2.2. Injection takes place at the bottom of the coal seam from the tip of a horizontal injection well. Production takes place via a vertical production well which is completed over the entire height of the coal layer. There are four subregions: the ash region $\Omega_A$, the coal region $\Omega_C$, the void region $\Omega_V$, and the roof-rock region $\Omega_R$. The gasified region $\Omega_A$, in which
all coal has been consumed, consists of ash and spalled rock. No distinction is made between ash and spalled rock. The downstream coal region $\Omega_C$ contains unreacted coal and char. We disregard heat losses and assume that $\Omega_C$ has a constant (produced gas-) temperature.

There are four interfaces. $\Gamma_{vr}$ is the interface between the rock and the void. $\Gamma_{vc}$ and $\Gamma_{ac}$ are the interfaces between void and coal, and between ash and coal, respectively. $\Gamma_{vc} \cup \Gamma_{ac}$ is the interface between the gasified regions $\Omega_A \cup \Omega_V$ and the coal region $\Omega_C$. Finally, $\Gamma_{va}$ is the interface between void region $\Omega_V$ and ash region $\Omega_A$. We use the term cavity to denote the total void space. The whole domain consisting of ash, char, coal, rock, and void, is indicated by $\Omega$.

### 2.2.2 Flow modelling

The underground reactor represented by the domain $\Omega$ is modelled as a heterogeneous permeability field. The flow is governed by Darcy's equation. We disregard gravity effects resulting from small differences in gas density. Since only permeability ratios are important here, we measure all permeabilities by a reference quantity $k_{ref}$. We assign a permeability $k_{ref}$ to charred coal in the linkage zone. The virtually impervious nature of both unaffected coal and rock is modelled with a low permeability. The permeabilities of char, ash, and spalled rock are parameters of the model. Finally, the void is assigned a high permeability, to model a constant pressure condition.

The injection and production boundary conditions are a constant injection rate and a constant production pressure, respectively. In the flow model we distinguish two temperature regions: an upstream region, $\Omega_A \cup \Omega_R \cup \Omega_V$, controlled by the injection temperature and a downstream region, $\Omega_C$, controlled by the produced gas temperature. The actual cavity temperatures are in fact very much
higher than the injection temperature, but the high permeability of the cavity entirely determines the flow inside the cavity. The temperature dependencies of the gas viscosities are given by [6]: \( \mu_\infty / \mu_d = (T_\infty / T_d)^{0.634} \). We disregard the composition dependence of the gas viscosity \( \mu \). More sophisticated approximations are not warranted in view of the uncertainty of the permeability distribution.

The flow equations are solved using a probabilistic method. Probabilistic methods were introduced for problems in reservoir engineering by Patterson [7] who showed the analogy between diffusion-limited aggregation (DLA) of colloids and flow in porous media. Both processes are described by Laplace's equation, with similar boundary conditions. DeGregoria [8] and King and Scher [9] extended the DLA approach to complex flow problems in porous media.

King [10] has shown that the probabilistic method gives similar results as deterministic methods for a variety of stable displacement processes. King's work is based on a stream-function approach. Frick et al. [11] use a pressure formulation. Probabilistic methods are highly suitable for unstable displacements. For stable displacements a deterministic solution method should lead to essentially the same results.

### 2.2.3 Cavity gasification by surface reactions

The coal surface of the cavity reacts with the gases in the cavity. At sufficiently high temperatures, the coal consumption rate is determined by the mass transfer rate through the boundary layer between the coal and the cavity. The mass transfer in turn is controlled by natural convection. The forced convection flows in the cavity can be ignored [12].

In the Chapters 3 and 4 it is shown that a uniform mass-transfer rate gives a reasonable estimate for natural-convection-driven coal-surface gasification. For turbulent natural convection flows, i.e., at high Rayleigh numbers (\( Ra \geq 1 \cdot 10^{18} \)), the transfer rate is estimated by: \( k_f \left[ m^3 / m^2 s \right] = 280 \ D \), in which \( D \left[ m^2 / s \right] \) denotes the molecular diffusion coefficient. The value of \( k_f \) is distributed relatively uniformly over the cavity boundary [13]. The reaction rate \( r \left[ \text{kg carbon} / m^2 s \right] = k_f P \ [O_2] M_c \), in which \( [O_2] \) is the molar oxygen concentration. The composition in the cavity may differ from the injection composition, but this will be disregarded as oxygen is replaced by carbon dioxide which also reacts with the coal wall.

### 2.2.4 Permeable-bed gasification reactions

Prior to gasification, a link, i.e., a permeable path is made in the coal zone between the injection well and the production well. After linkage, a cavity starts to develop at the point where air or air enriched with oxygen is injected, see Fig. 2.2. Part of the permeable-bed gasification takes place at the ash coal interface (\( T_{ae} \)). Here the injected gas reacts directly with the permeable coal. The
other part reacts indirectly at the void/coal interface ($\Gamma_{vc}$). By direct reaction we mean that the injected gas only reacts with coal and does not enter the cavity. Part of the gas, however, reacts indirectly with the coal: gas, that enters the cavity with injection composition and temperature, reacts with the omnipresent combustible gases to form hot combustion products, e.g. CO$_2$ and H$_2$O.

Part of the combustion products and remaining oxygen (if there is insufficient combustible gas) reacts at the coal wall driven by natural convection flows (cavity gasification; see below). The other part reacts with the coal between the cavity wall through which it is flowing and the production well (indirect permeable-bed gasification).

In spite of this, we make no distinction between direct and indirect permeable-bed gasification. We merely use a parameter ($P$) to define how many carbon atoms react with one molecule of oxygen (O$_2$).

As a result of the reactions, the mass flux increases by addition of coal atoms to the gas. If gas reacts indirectly we can (owing to the high cavity permeability) assume that the entire increase in mass flux is concentrated at the interface $\Gamma_{vc}$ without affecting the flow field. We assume a constant composition of the produced gas. Thus the ratio of the mass flux downstream and the mass flux upstream of the interfaces $\Gamma_{vc} \cup \Gamma_{ac}$ is constant. Furthermore, we assume ideal gas behaviour. The temperature of the produced gas is the adiabatic flame temperature.

### 2.2.5 Coal and roof failure

Three mechanisms of roof failure are distinguished, viz. rock/coal spalling, melting and large-scale roof collapse as a result of stress concentrations near the side boundaries of the cavity. Large-scale roof collapse takes place when a considerable section of the roof is unsupported. The critical span depends on the rock-mass properties of the roof. The effect is less important at the initial stages of the gasification process and has not been taken into account.

Spalling is chipping of rock induced by thermal and mechanical stresses [14]. Spalling occurs in both coal and rock. High spall rates develop only in rock/coal exposed to cavity temperatures exceeding 500°C [15]. The high temperature and pressure inside the cavity cause spalled coal blocks are to be gasified immediately [5]. We assume that spalling takes place at a constant and spatially uniform rate. Spalling is introduced in the model as a local phenomenon. The spall locations are determined at random. The volume of spalled rock/coal per unit original rock/coal volume are model parameters. The spall rates for rock and coal are model parameters. Melting effects can be modelled with increased spall rates and a low permeability of the chipped rock.

Once a block of coal is gasified, its ash is added to the ash/rock rubble pile directly below it. This ash/rubble pile is subsequently redistributed according to its angle of repose. For this study, we take the angle of repose to be 30 degrees.
2.2.6 Cavity evolution

The procedure to determine the cavity evolution is as follows: let the spatial distribution of ash, void, char, and coal be given at a certain time. This geometry defines the permeability distribution. At the beginning of a time step, we determine the flow field by applying Darcy’s equation for the given permeability distribution. Because the coal consumption rate is small with respect to the gas velocities we can assume stationary flow conditions. We then calculate the change in spatial distribution of ash, void, char, and coal during the time step. Coal is consumed at the interfaces $\Gamma_{vc} \cup \Gamma_{ac}$ at a rate proportional to the normal flux at the interface. At the cavity boundary an extra amount of coal is gasified as a result of natural-convection-driven surface gasification. The volume of gasified coal becomes void space which is added to the cavity, and its ash falls to the bottom of the cavity. The ash-void interface $\Gamma_{va}$ moves downward when the coal beneath it is gasified. The rock and coal exposed to the cavity spall at a constant rate and also fall down vertically. Given the new spatial distribution we then update the permeability distribution and the calculation procedure is repeated for the next time step.

2.3 Model equations

2.3.1 Generalized mass-flux vector

A generalized mass-flux vector $\vec{j}$ is defined by

$$\vec{j} = m \rho \vec{q}$$

$$\left\{ \begin{array}{l}
\frac{m}{\chi} = \frac{1}{\chi} & \text{in } \Omega_C \\
\frac{m}{1} = m & \text{in } \Omega_A \cup \Omega_R \cup \Omega_V
\end{array} \right. \quad (2.1)$$

in which $\vec{q}$ is the specific discharge and $\rho$ is the density of the gas. The ratio $\chi$ between the mass flux downstream $(\rho q)_{C,n}$, and the mass flux upstream $(\rho q)_{A/V,n}$ of the interface between $\Omega_A \cup \Omega_V$ and $\Omega_C$ is constant. A similar ratio can also be defined in steam drive [16], and filtration gasification [17]. The (stationary) conservation law reads $\text{div } \vec{j} = 0$ in the whole domain $\Omega$ or

$$\begin{align*}
\text{div } \vec{j} &= 0 & \text{in } \Omega \\
j_{A,n} &= j_{C,n} & \text{on } \Gamma_{ac} \\
j_{V,n} &= j_{C,n} & \text{on } \Gamma_{vc}
\end{align*} \quad (2.2)$$

in which $j_{A,n}$ and $j_{V,n}$ are the normal components of the upstream generalized mass-flux vector at $\Gamma_{vc}$ and $\Gamma_{ac}$, respectively, and $j_{C,n}$ is the downstream generalized mass flux. Note that $(\rho q)_{A,n} \neq (\rho q)_{C,n}$ and $(\rho q)_{V,n} \neq (\rho q)_{C,n}$. 
2.3. MODEL EQUATIONS

2.3.2 Darcy equation and pressure equation

Substitution of Darcy’s equation in Eq. 2.1 gives

$$\bar{j} = -\rho \frac{k m}{\mu} \text{grad} p \quad \text{in } \Omega.$$  \hspace{1cm} (2.3)

The viscosity has two different values, viz. $\mu_u$ in the upstream region ($\Omega_u \cup \Omega_r \cup \Omega_V$) and $\mu_d$ in the downstream region ($\Omega_C$). Substitution of Eq. 2.3 into Eq. 2.2 leads to the pressure equation

$$\text{div} \frac{\rho k m}{\mu_d} \text{grad} p = 0 \quad \text{in } \Omega_C$$  \hspace{1cm} (2.4)

$$\text{div} \frac{\rho k m}{\mu_u} \text{grad} p = 0 \quad \text{in } \Omega_u \cup \Omega_r \cup \Omega_V$$

Because we introduced the generalized mass-flux vector, we can derive one single pressure equation for the whole domain. The boundary conditions are the prescribed injection rate at the injection well, the constant production pressure and the no-flow boundary conditions at the outer boundary of the domain $\Omega$. Once the pressure field is known we can determine the flow field $\bar{j}$ at the interfaces $\Gamma_{vc} \cup \Gamma_{ac}$ by the application of Darcy’s equation, Eq. 2.3.

2.3.3 Cavity development

We assume that the interfaces can be written as a function of the x- and y-coordinates, i.e., $\gamma_{\alpha\beta} = \gamma_{\alpha\beta}(x, y, t)$ in which $\gamma_{\alpha\beta}$ denotes the z-coordinate of the interface between $\Omega_\alpha$ and $\Omega_\beta$, with $\alpha, \beta = \text{ash, coal, void, rock}$. The interface heights $\gamma_{\alpha\beta}(x, y, t)$ are only defined for those values of $x$ and $y$ that are physically relevant. The equations of motion of the interfaces read

$$\begin{align*}
\frac{\partial \gamma_{\text{tr}}}{\partial t} &= \frac{\lambda_{\text{rock}}}{a_{\text{tr}}} \quad \text{on } \Gamma_{\text{tr}} \\
\frac{\partial \gamma_{\text{vc}}}{\partial t} &= \frac{\omega(\rho q) & \nu_{\gamma_{\text{vc}}} + \frac{P k_f M_{\text{coal}} k_{\text{fl}}}{\rho_{\text{coal}}}}{a_{\text{vc}}} + \frac{\lambda_{\text{coal}}}{a_{\text{vc}}} \quad \text{on } \Gamma_{\text{vc}} \\
\frac{\partial \gamma_{\text{ac}}}{\partial t} &= \frac{1}{a_{\text{ac}}} \omega(\rho q)_{\gamma_{\text{ac}}} \quad \text{on } \Gamma_{\text{ac}} \\
\frac{\partial \gamma_{\text{oa}}}{\partial t} &= \zeta \frac{\partial \gamma_{\text{tr}}}{\partial t} + \nu \frac{\partial \gamma_{\text{vc}}}{\partial t} + (1 - \nu) \frac{\partial \gamma_{\text{ac}}}{\partial t} \quad \text{on } \Gamma_{\text{oa}} \end{align*}$$  \hspace{1cm} (2.5)

In Eq. 2.5 the terms $\lambda_{\text{rock}}$ and $\lambda_{\text{coal}}$ represent the spalling of rock and coal, respectively. The factor $a_{\alpha\beta}$ denotes the projected area onto a horizontal plane.
of one unit of exposed surface. The terms $\omega(\rho q)_{A,n}$ and $\omega(\rho q)_{V,n}$ denote the coal that is gasified as a result of permeable-bed gasification reactions and $(\rho q)_{V,n}$ is the mass flux perpendicular to $\Gamma_{\text{ec}}$, i.e., the cavity/coal interface. $(\rho q)_{A,n}$ is the mass flux perpendicular to $\Gamma_{\text{ac}}$, i.e., the ash/coal interface. $\omega$ is the volume of coal gasified per unit mass of gases, and is proportional to $P$, the number of moles carbon that are affected by a mole of oxygen.

The term $P k_f \frac{M_c}{\rho_{\text{coal}}} \frac{f P}{RT}$ represents the coal that is gasified owing to the natural convection of gases in the cavity, $f$ denotes the fraction of oxygen in the injection gas, $\rho_{\text{coal}}/M_c$ is the molar density of coal, and $\frac{f P}{RT}$ is the molar concentration of oxygen in the injection gas.

$\frac{\partial \rho_{\text{coal}}}{\partial t}$ consists of positive terms resulting from the spalling of rock and ash originating from the spalled/gasified coal, and a negative term resulting from gasification underneath it. $\nu$ is the volume of ash per unit volume of coal gasified. $\zeta$ represents the volume of spalled rock at the cavity floor that originates from a unit volume of roof rock.

2.4 Numerical model

The numerical model calculates the pressure field at successive time steps. In our example domain the bottom half of the reactor consists of coal and the top half of roof rock. At each time step we calculate the pressure field (see Appendix 2A), and from it the generalized mass-flux field. Once the flow field is calculated the cavity development for a single time step is determined. To this end we could use the mass fluxes normal to the void/coal interface $\Gamma_{\text{vc}}$ and the ash/coal interface $\Gamma_{\text{ac}}$ directly in the equation of motion, Eq. 2.5, but a deterministic approach does not recognize the possibly unstable character of this process. The advantage of the probabilistic method adopted here is that it constantly perturbs the solution. Therefore the probabilistic method readily detects unstable situations by giving different answers for different realisations [17]. In deterministic simulators noise has to be introduced to create unstable behaviour [18].

The procedure to determine the cavity development for a single time step is as follows: first we calculate the total flow, $Q$, from non-coal locations through all coal/char faces which are exposed to either void or ash, see also Fig. 2.3. Then we use a random-number generator [19] to draw a single random number, $R_1$, uniformly distributed between zero and one. Subsequently, we repeat the summation through the exposed coal/char faces until the value $R_1 Q$ is reached. At this location, the block of char or coal is gasified and a corresponding amount of ash is released. The ash falls down and accumulates at the bottom of the cavity.

At specific intervals, depending on the coal spall rate, a second and third random number are drawn. These random numbers specify the $(x,y)$ location (column) of a coal block, which can spall if there is cavity directly below it. In
2.4. **NUMERICAL MODEL**

![Coal/char](image)

Figure 2.3: From a single void or ash location (centre cube) all flows through each of the cube's faces are added, if the adjacent blocks are char or coal.

This way, the coal spall rate is made proportional to the exposed coal surface. The spalled coal block is gasified immediately [5], its ash content is released, falls down and accumulates at the bottom of the cavity. Two other random numbers select a block of rock for spalling. It should again be noted that only blocks of rock the surfaces of which are exposed to the cavity can spall. Indeed, in the early stages of cavity growth no rock can spall. The spalled rock is released, falls down and accumulates as “ash” at the bottom of the cavity. An expansion factor can be assigned to the spalled material, to account for its increase in porosity.

Finally, a small portion of the coal surface that is exposed to the cavity is removed to account for the surface gasification. The ensuing ash accumulates at the bottom of the cavity. We accommodate the void/ash interface to the condition that no void space exists below the ash. The ash and rock rubble are finally redistributed according to the angle of repose. With the updated cavity a new pressure field is calculated and the new velocities are determined. Subsequently, the cavity development is determined for the next time step, etc.

### 2.4.1 Iterative solution of pressure equation

The pressure equation is a 3D elliptic equation that has to be solved at every time step. In the model we use the multigrid method that was developed by Molenaar (for details, see [20, 21]). The amount of computational work that multigrid solvers require is proportional to the number of grid points. This property makes them potentially superior to other iterative methods. In a multigrid method a hierarchy of discretization grids with increasing resolution is used. In order to solve the pressure equation we use a cell-centered multigrid method in which each of the coarse-grid cells is the union of four fine-grid cells. The high frequency error
components on the finest grid are efficiently reduced by means of a Gauss-Seidel relaxation method. The low frequency error components are reduced by using a correction that is calculated on a coarser grid. This coarse-grid problem is approximated by a combination of relaxation sweeps and corrections using even coarser grids (recursion). For our pressure equation, with strong variations in permeability, the multigrid method turns out to be an efficient and robust solver.

2.5 Example calculations

2.5.1 Introduction

To illustrate the model we present some example 3D calculations for a UCG reactor represented by a 16×16×16 grid. The grid consists of eight coal layers on the bottom. On top of the eight coal layers are eight layers of a roof rock that has a low permeability. A schematic diagram of the initial simulation domain is shown in Fig. 2.1. An aspect ratio \( h/L = h/W = 1/2 \) was used. A coal-layer thickness of 4 metres is considered throughout our example calculations.

The example calculations investigate the influence of ash permeability, and of coal and rock spall rates on the growth of an underground gasification cavity. For all cases but one (Case G) it is assumed that the whole coal zone was charred prior to (forward) gasification, resulting in a permeability that equals \( k_{ref} \) in the entire coal zone. Other realizations (with different seeds for the random-number generator) show qualitatively the same behaviour as the results presented below. The configuration used is considered to be representative for the first CRIP manoeuvre.

2.5.2 Input data

The input values for the base case simulation are shown in Table 2.1. For each time step, \( N \) pairs of random numbers \( R_2 \) and \( R_3 \) are drawn to obtain possible coal spalling sites. This leads to a coal spall-rate probability for one column (out of the 256 columns \( h \Delta x \Delta y \)) of \( \frac{N}{256} \) per gasified coal block. A high spall rate corresponds to a high value of \( N \). Spalling from the roof can take place if the column intersects the cavity. The average spall rate for rock was taken to be equal to the average coal spall rate for all cases considered. Figures 2.4 to 2.11 show the calculation results for a 16×16×16 grid. In the figures, only the bottom (coal) half is shown in a 3D view. The ash region that forms at the bottom of the cavity during the simulations is omitted as well, for reasons of clarity. The injection/production well layout is shown schematically in Fig. 2.1. Table 2.2 lists the remaining input parameters which were used for each of the Cases A to G.
Table 2.1: Base case input parameters.

<table>
<thead>
<tr>
<th>Constant</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$</td>
<td>$2.6 \cdot 10^{-4}$</td>
<td>m²/s</td>
</tr>
<tr>
<td>$f$</td>
<td>0.21</td>
<td>–</td>
</tr>
<tr>
<td>$h \times L \times W$</td>
<td>$4 \times 8 \times 8$</td>
<td>m³</td>
</tr>
<tr>
<td>$k_f$</td>
<td>$2.8 \cdot 10^{-3}$</td>
<td>m³/m²s</td>
</tr>
<tr>
<td>$k_{ref}$</td>
<td>1</td>
<td>mD</td>
</tr>
<tr>
<td>$k_{ash}$</td>
<td>1</td>
<td>$k_{ref}$</td>
</tr>
<tr>
<td>$k_{coal}$</td>
<td>1</td>
<td>$k_{ref}$</td>
</tr>
<tr>
<td>$k_{rock}$</td>
<td>$1 \cdot 10^{-3}$</td>
<td>$k_{ref}$</td>
</tr>
<tr>
<td>$k_{void}$</td>
<td>$1 \cdot 10^5$</td>
<td>$k_{ref}$</td>
</tr>
<tr>
<td>$M_c$</td>
<td>0.012</td>
<td>kg/mole</td>
</tr>
<tr>
<td>$p$</td>
<td>$5 \cdot 10^6$</td>
<td>Pa</td>
</tr>
<tr>
<td>$P$</td>
<td>2</td>
<td>mole/mole</td>
</tr>
<tr>
<td>$q_{inj}$</td>
<td>$1.65 \cdot 10^5$</td>
<td>¹standard m³/day</td>
</tr>
<tr>
<td>$r$</td>
<td>$1.41 \cdot 10^{-4}$</td>
<td>kg/m²s</td>
</tr>
<tr>
<td>$T_d$</td>
<td>1673</td>
<td>K</td>
</tr>
<tr>
<td>$T_u$</td>
<td>313</td>
<td>K</td>
</tr>
<tr>
<td>$\mu_u / \mu_d$</td>
<td>0.35</td>
<td>–</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.5</td>
<td>m³/m³</td>
</tr>
<tr>
<td>$\rho_c$</td>
<td>1300</td>
<td>kg/m³</td>
</tr>
<tr>
<td>$\zeta$</td>
<td>1.0</td>
<td>m³/m³</td>
</tr>
<tr>
<td>$\chi$</td>
<td>1.14</td>
<td>kg/kg</td>
</tr>
</tbody>
</table>

¹standard conditions: $1 \cdot 10^5$ Pa, 293 K
Table 2.2: Variation in input parameters for example calculations.

<table>
<thead>
<tr>
<th>Case</th>
<th>Spall rate [-]</th>
<th>$k_{\text{ash}}$ $[k_{\text{ref}}]$</th>
<th>$k_{\text{coal}}$ $[k_{\text{ref}}]$</th>
<th>$k_{\text{rock}}$ $[k_{\text{ref}}]$</th>
<th>$k_{\text{void}}$ $[k_{\text{ref}}]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>21/256</td>
<td>1</td>
<td>1</td>
<td>$10^{-3}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>B</td>
<td>0</td>
<td>$10^5$</td>
<td>1</td>
<td>$10^{-3}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>C</td>
<td>50/256</td>
<td>$10^5$</td>
<td>1</td>
<td>$10^{-3}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>D</td>
<td>0</td>
<td>$10^{-3}$</td>
<td>1</td>
<td>$10^{-3}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>E</td>
<td>50/256</td>
<td>$10^{-3}$</td>
<td>1</td>
<td>$10^{-3}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>F</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>G</td>
<td>0</td>
<td>1</td>
<td>$10^{-3}$</td>
<td>$10^{-3}$</td>
<td>$10^5$</td>
</tr>
</tbody>
</table>

1 A highly permeable $(10^5 k_{\text{ref}})$ zone links injector and production well

Table 2.3: Sweep efficiency at the point in time where the cavity reaches the production well. Calculations for the base case with four combinations of ash permeability and spall rate for coal and rock.

<table>
<thead>
<tr>
<th>$k_{\text{ash}}$ $[k_{\text{ref}}]$ spall rate [-]</th>
<th>Sweep of 100 realisations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>avg</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>0</td>
</tr>
<tr>
<td>50/256</td>
<td>0.640</td>
</tr>
<tr>
<td>$10^{-3}$</td>
<td>5/256</td>
</tr>
<tr>
<td>$10^5$</td>
<td>50/256</td>
</tr>
</tbody>
</table>

2.5.3 Effect of random number seed

Since we use a probabilistic approach to determine both cavity evolution and coal and roof failure, we have carried out a number of calculations with variations in seeds for the random-number generator. The results of these calculations on a 16x16x16 grid are shown in Table 2.3. For the seed variation calculations, we used the base case with four combinations of ash permeability and spall rate. These two parameters were found to have the most profound influence on cavity geometry and sweep efficiency. The results lead to the conclusions that for all cases considered here, different seeds for the random-number generator result in a low variance of sweep efficiency at breakthrough in the production well. The average sweep efficiencies are generally high, but the combination of a low ash permeability with no spalling leads to a low (average) sweep. In general, we can conclude that the number of gridblocks is large enough to ensure a low variance in the results.
2.5.4 Base case

The base case, A, see Fig. 2.4, with an average spall rate of \((21/256)\) and an ash permeability of \((k_{\text{ref}})\), shows a slightly asymmetrical cavity that has developed in the coal region, after 40% of the coal has been gasified. The ash/rock rubble pile that is formed around the injection point, (not shown in the figure) covers part of the coal surface, inhibiting the cavity surface gasification process (since this coal is not exposed to the void space). This results in the cavity growing more rapidly towards the top of the coal layer, since coal is eaten away faster there. In addition, the spalling process also causes the cavity to grow upwards, towards the overburden.

2.5.5 Effect of natural-convection-driven surface gasification

Figure 2.5 shows the fraction of the coal initially in place that was gasified as a result of natural-convection-driven surface gasification, and the fraction of the coal that was gasified as a result of direct gasification (including coal spalling), plotted versus the total amount of coal gasified. The figure clearly shows that, in the base case, surface gasification and direct gasification are comparable in size. After approximately 18% of the coal initially in place has been gasified, surface gasification becomes more important than direct gasification. The high ash percentage (50%), however, prevents large parts of the coal's surface to become exposed and contribute to the surface gasification process. This is the reason why the difference between surface and direct gasification remains more or less constant for the remainder of the simulation.

2.5.6 Effect of spalling

Figures 2.6 and 2.7, Cases B and C, show a 3D view of the gasified region, without spalling and with considerable spalling, respectively. Both cases have the same (high) ash permeability and ash content. Figure 2.6 (Case B) shows an evenly developed cavity which has grown steadily upwards to the low permeable roof rock (not shown in the picture). In contrast, Fig. 2.7 shows a cavity which has grown mostly to one side of the simulation domain. The cavity has very steep walls as a result of the high spall rates. Figures 2.8 and 2.9, Cases D and E, show the influence of spalling on cavity development when ash permeabilities are very low, \(10^{-3}k_{\text{ref}}\). Case D, without spalling, shows a cavity which formed mainly low in the coal region and spread widely. Case E, with a high spall rate, shows a cavity with an irregular shape with steep coal walls, and a large coal zone in the centre of the region which is bypassed.
Figure 2.4: Case A: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 21/256, ash permeability is $k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1.

Figure 2.5: Case A: fraction of coal initially in place gasified as a result of surface gasification and coal gasified as a result of direct gasification (permeable-bed gasification and coal spalling) versus the total amount of coal gasified.

2.5.7 Effect of ash permeability

Figures 2.6 to 2.9 demonstrate the effect that ash permeability has on the gasification process. Cases B and D show that, when the spall rate is zero, the ash
2.5. EXAMPLE CALCULATIONS

Figure 2.6: Case B: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 0, ash permeability is $10^5 k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1.

Figure 2.7: Case C: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 50/256, ash permeability is $10^5 k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1.

permeability indeed has a profound influence on cavity development. In Case B high ash permeability ($10^5 k_{ref}$) leads to a cavity which develops more or less symmetrically around the injection point. The flow of gases is not hindered by the ash/rock rubble pile. Cavity-surface gasification only takes place at the exposed coal surface, causing the upper part of the cavity to grow faster. Case D, with a low ash permeability ($10^{-3} k_{ref}$), shows a highly irregular cavity shape as a result of the blocking of the injected gas by the ash/rock rubble pile. The layered
Figure 2.8: Case D: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 0, ash permeability is $10^{-3}k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1.

Figure 2.9: Case E: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 50/256, ash permeability is $10^{-3}k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1.

structure of the ash pile keeps most of the cavity low in the coal region.

For a high spall rate (50/256) Case C (viz. Fig. 2.7) shows that a high ash permeability ($10^3k_{ref}$), leads to an asymmetrical cavity with steep walls as a result of the high spall rate. By contrast, Case E (see Fig. 2.9) with a low ash permeability ($10^{-3}k_{ref}$) leads to a cavity, that has with steep walls as well, but is developed more evenly in the coal region.
2.5. EXAMPLE CALCULATIONS

Figure 2.10: Case F: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 0, ash permeability is $k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1.

2.5.8 Effect of a homogeneous permeability field

Case F, Fig. 2.10, shows the cavity developed for a homogeneous permeability field. Here, a more or less symmetrical cavity develops without influence of ash permeability or spall rate.

2.5.9 Effect of a limited linkage zone

In Case G, Figs 2.11 and 2.12, the influence of a band-like linkage zone of high permeability connecting injector and production well is studied. This is an idealized representation of a link obtained by reverse combustion or hydraulic fracturing.

Figure 2.11 shows that a symmetrical cavity develops in the coal, which concentrates mainly around the high-permeability linkage zone. Figure 2.12 shows two pictures of the 3D velocity field inside the domain. The high-permeability linkage zone ($10^5 k_{ref}$) at $W/2$ is indicated by a narrow band of lines around the coal domain. The left picture shows the initial velocity field, the one on the right shows the velocity field after 40% of the coal has been gasified. The difference in velocity distribution is due mainly to the fact that a void space with a very high permeability ($10^5 k_{ref}$) has formed, leading to a more even velocity distribution, and higher velocities higher up in the cavity. Another aspect is that when coal near the linkage zone is gasified, a corresponding amount of ash is released, and falls down, effectively blocking the flow path below it. This also causes the cavity to grow upwards.
Figure 2.11: Case G: 3D view showing the gasified region, after 40% of the coal has been gasified. The spall rate is 0, ash permeability is $k_{ref}$, and ash content is 50%. The injection/production well layout is shown in Fig. 2.1. At W/2 a highly permeable region links injector and production well.

Figure 2.12: Case G: Two 3D views from the side (injection point at the left of the domain, production line at the right) showing the initial velocity distribution in the left picture, and the velocity distribution after 40% of the coal has been gasified in the right picture. The vertical highly permeable linkage zone at W/2 is indicated with a band around the coal domain. The two large arrows in each of the pictures indicate the high velocities near the injection point.
2.6 Conclusions

- We have developed a 3D model for underground coal gasification which incorporates natural-convection-driven coal surface gasification and permeable-bed gasification as well as temperature- and stress-induced failure of both rock and coal.

- In order to be able to apply the model to practical field cases, experimental data are required on reaction mechanisms and (local) mass transfer rates.

- Thermo-mechanically induced spalling appears to be an important mechanism in underground coal gasification. Therefore, the physics of the processes which control spalling should be investigated in detail.

- The example calculations presented in this chapter generally show a fairly high sweep efficiency, indicating that the CRIP process is very efficient for a wide range of input parameters.

- Natural convection contributes significantly to the total amount of gasified coal.
Nomenclature

Latin

\( a \) = projected area on a horizontal plane
\( D \) = molecular diffusion coefficient, \( \text{L}^2 / \text{t}, \text{m}^2 / \text{s} \)
\( f \) = oxygen fraction in injection gas
\( h \) = height of coal layer, \( \text{L}, \text{m} \)
\( j \) = mass flux, \( \text{m} / \text{L}^2 \text{t}, \text{kg} / \text{m}^2 \text{s} \)
\( j \) = mass flux vector, \( \text{m} / \text{L}^2 \text{t}, \text{kg} / \text{m}^2 \text{s} \)
\( k \) = permeability, \( \text{L}^2, \text{m}^2 \)
\( k_f \) = mass transfer rate constant, \( \text{L}^3 / \text{L}^2 \text{t}, \text{m}^3 / \text{m}^2 \text{s} \)
\( K \) = averaged conductivity tensor, \( \text{t}, \text{s} \)
\( L \) = length of coal layer, \( \text{L}, \text{m} \)
\( m \) = normalization factor
\( M \) = molecular mass, \( \text{m} / \text{mole}, \text{kg} / \text{mole} \)
\( N \) = number of pairs of random numbers
\( p \) = pressure, \( \text{m} / \text{Lt}^2, \text{Pa} \)
\( P \) = mole carbon/mole \( \text{O}_2 \)
\( q_{\text{inj}} \) = injection rate, \( \text{L}^3 / \text{t}, \text{m}^3 / \text{day} \)
\( Q \) = total flow rate, \( \text{L}^3 / \text{t}, \text{m}^3 / \text{s} \)
\( q \) = specific discharge, \( \text{L} / \text{t}, \text{m} / \text{s} \)
\( r \) = reaction rate, \( \text{m} / \text{L}^2 \text{t}, \text{kg} / \text{m}^2 \text{s} \)
\( R \) = gas constant, \( \text{m} \text{L}^2 / \text{t}^2 \text{T}, \text{J} / \text{mole K} \)
\( \mathcal{R} \) = random number
\( Ra \) = Rayleigh number
\( t \) = time, \( \text{t}, \text{s} \)
\( t_p \) = project time, \( \text{t}, \text{days} \)
\( T \) = temperature, \( \text{T}, \text{K} \)
\( W \) = width of coal layer, \( \text{L}, \text{m} \)

Greek

\( \gamma \) = interface height, \( \text{L}, \text{m} \)
\( \Gamma \) = interface
\( \lambda \) = spall factor, \( \text{L} / \text{t}, \text{m} / \text{s} \)
\( \mu \) = dynamic viscosity, \( \text{m} / \text{Lt}, \text{Pa}\cdot\text{s} \)
\( \nu \) = volume ash/volume coal, \( \text{L}^3 / \text{L}^3, \text{m}^3 / \text{m}^3 \)
\( \rho \) = density, \( \text{m} / \text{L}^3, \text{kg} / \text{m}^3 \)
\( \zeta \) = volume ash/volume rock, \( \text{L}^3 / \text{L}^3, \text{m}^3 / \text{m}^3 \)
\( \chi \) = mass flux ratio, \( \text{m} / \text{m}, \text{kg} / \text{kg} \)
\( \omega \) = volume coal gasified by a unit mass gas, \( \text{L}^3 / \text{m}, \text{m}^3 / \text{kg} \)
2.6. CONCLUSIONS

\[ \Omega = \text{domain} \]

\textbf{Subscripts}

- \( A \) = ash region
- \( ac \) = ash/coal
- \( c \) = coal
- \( C \) = coal region
- \( d \) = downstream
- \( n \) = normal vector component
- \( r \) = rock
- \( R \) = roof-rock region
- \( ref \) = reference
- \( u \) = upstream
- \( V \) = void region
- \( va \) = void/ash
- \( vc \) = void/coal
- \( vr \) = void/rock
- \( x \) = x-direction (horizontal)
- \( y \) = y-direction (horizontal)
- \( z \) = z-direction (vertical)
Bibliography


Appendix 2A

Solution of the equation of motion

The procedure described here is an extension of the procedure given by King [10]. The domain is subdivided in $N_x \times N_y \times N_z$ grid blocks of size $\Delta x \times \Delta y \times \Delta z$. In the calculations shown we use cubical grid blocks ($\Delta x = \Delta y = \Delta z$). Each grid block may contain a few horizontal layers of e.g. coal, rock, charred coal, void, or ash/spalled rock. The different components (coal etc.) are indicated in Fig. 2.2. Most grid blocks contain a single component. Grid blocks in the vicinity of the interfaces $\Gamma_{ac}$ and $\Gamma_{ve}$, however, may consist of two and in some cases three components. Void cannot be overlain by ash and spalled rock.

The approximate interface heights $\tau_{ac}(x, y, t_l)$ are piecewise constant on the square with corners $(n \Delta x, m \Delta y)$ and $((n+1)\Delta x, (m+1)\Delta y)$, $m=0,1,..., n=0,1,...$, and calculated for times $t_l$, $l=0,1,...$. In each time step $\Delta t_l= t_{l+1} - t_l$ the following events take place. First, a coal block of volume $\Delta x^3$ is gasified. Secondly, a certain amount of coal is gasified by cavity gasification. Thirdly, a coal block may spill and is subsequently gasified. Finally, a piece of rock may spill. The time $\Delta t_l$ is calculated from the air injection rate and the amount of coal gasified. As a result of these events the interface height $\tau_{ac}(x, y, t_{l+1})$ is determined from the interface height $\tau_{ac}(x, y, t_l)$ as follows. First we calculate the total flow, $Q$, through all coal/char faces which are exposed to either void or ash. Then we use a random number generator [19] to draw a single random number, $R_{11}$, uniformly distributed between zero and one. Subsequently, we repeat the summation through the exposed coal and char faces until the value $R_{1}Q$ is reached. The coal block nearest to the intersection point with height $\Delta x$ is removed. Either the interface $\tau_{ac}$ is lowered by $\Delta x$ or the interface $\tau_{ve}$ is moved up by $\Delta x$ at this position. The coal near the interfaces $\tau_{ac}$ and $\tau_{ve}$ that have the highest mass flux has the highest probability to be gasified. This method is based on the fact that the velocity values plotted along the interface can be interpreted as a cumulative distribution function [10,19]. The interface $\tau_{ve}$ is further moved as a result of natural-convection-driven cavity gasification in a deterministic fashion: all hori-
zontal faces of \( \tilde{\gamma}_{vc} \) are moved upward by an amount proportional to the added coal surfaces of the block under consideration and all exposed blocks vertically above it. The constant of proportionality is the natural-convection-driven transfer rate \( r/\rho_{coal}\Delta t_i \).

A second and third random number \( R_2 \) and \( R_3 \) are drawn and multiplied by \( L \) and \( W \), respectively, at specific intervals within each time step, depending on the coal spall rate. \( (R_2 L, R_3 W) \) is an \( x, y \)-location that specifies a column of grid blocks. If this column intersects with \( \Gamma_{vc} \) it indicates a position where coal spalling takes place. The interface \( \tilde{\gamma}_{vc} \) at the position of the column is moved upwards by \( \Delta x \). A fourth and fifth random number \( R_4 \) and \( R_5 \) are drawn at specific intervals, depending on the rock spall rate. \( (R_4 L, R_5 W) \) is an \( x, y \)-location that specifies a column of \( N_z \) grid blocks. If this column intersects with \( \Gamma_{vr} \), it indicates a position where rock spalling takes place. The interface \( \tilde{\gamma}_{vr} \) at the position of the column is moved upward by \( \Delta x \). Finally, \( \tilde{\gamma}_{va} \) is moved as a weighted sum of the movement of all other interfaces according to Eq. 2.5.

### 2A.1 Calculation of the flow field

Grid blocks have average permeability values. Therefore, we need an averaging procedure in each grid block for the conductivity \( \frac{\mu k m}{\mu} \). The averaged conductivity \( \mathbf{K} \) becomes a tensor. The horizontal (both the \( x \) and the \( y \)-direction) and vertical (the \( z \)-direction) conductivity values are arithmetic and harmonic averages respectively. Therefore the upscaled pressure Eq. 2.4 becomes

\[
\text{div } \mathbf{K} \cdot \text{grad} p = 0, \quad \text{in } \Omega. \tag{2A.1}
\]

\( \mathbf{K} \) has zero off-diagonal terms owing to the assumption that the permeability components form a horizontally layered structure.
Chapter 3

Temperature-driven natural convection

In this chapter we present laser Doppler measurements in a rectangular, differentially heated, enclosed convection chamber. The experimental results in the form of velocity and turbulent kinetic energy profiles are compared with numerical calculations. A low-Reynolds turbulence model shows the best agreement with the measurements.

3.1 Introduction

In underground coal gasification cavities or channels, natural convection flows form the most important mass transfer mechanism. The reason for this is that natural-convection flow velocities are much higher than any forced convection flow present [1] during UCG. Consequently, these turbulent natural convection flows will have significant influence on both cavity growth (see Chapter 2) and composition of the produced gas [2].

Theoretical studies [3] show that the shape of a cavity and its angle of inclination have a considerable effect on natural convection flows and heat- and mass-transfer rates. Few experimental data are available in the literature to validate the existing natural convection flow models, especially in the laminar/turbulent transition region. Recently, Opstelten [4] reported on experimental work investigating transition characteristics of natural convection flow in near-cubical, differentially heated cavities. In our study we use a rectangular (height-to-width ratio is 2), differentially heated convection chamber. The main difference between Opstelten's cubical cavity and our rectangular cavity [5] is not only the aspect ratio, but also the fact that our cavity can be tilted to a certain angle of inclination. Van Batenburg [5] reported earlier measurements, in which the rectangular cavity is placed under angles of 90 and 80 degrees with the horizontal, which agreed reasonably well with numerical results of Lankhorst [6].

The objectives of the experiments presented here are: (1) to validate the turbulence models that were used by Kuyper [3] for his underground coal-gasification
model, and (2) to determine the effect of the angle of inclination of the cavity, i.e., of its stage of development, on the character of natural-convection flows.

In this chapter, we present experimental results obtained with 2D laser Doppler velocimetry and compare them with numerical results. We will describe the experimental set-up: a rectangular convection chamber (schematically shown in Fig. 3.1). The rectangular set-up is heated differentially to induce natural convection flow.

![Diagram of rectangular convection chamber]

Figure 3.1: Schematic representation of the rectangular convection chamber.

### 3.2 Mathematical formulation

In this section we derive the system of equations that can be used to describe the flow inside the rectangular convection chamber. We first list the main assumptions that were used to derive the flow equations.

- The left and right walls of the rectangular chamber are each kept at a constant temperature $T_{\text{hot}}$ and $T_{\text{cold}}$, respectively. The top and bottom are
also kept at a constant temperature, without overall heat exchange. The front and back walls are insulated, to make the flow inside the chamber approximately two-dimensional at half the chamber depth \((D/2)\).

- We assume that the Navier Stokes equations apply with constant viscosity, and neglect variations in density as a result of pressure variations.

- The density changes caused by non-uniform heating result in forces which bring about natural convection.

- For the conservation of energy we use the equation of heat conservation, i.e., accumulation, convection, and conduction. Thermal conductivity is constant.

- The Boussinesq approximation is assumed to be valid, i.e. all fluid properties can be taken constant except for the density in the buoyancy term, which in turn can be linearised according to: \( \frac{\rho}{\rho_0} = 1 - \beta_T (T - T_{\text{ref}}) \), with \( \beta_T \) the thermal expansion coefficient.

Flow inside a cavity can be described by the continuity equation (conservation of mass), the Navier Stokes equations (conservation of momentum in the two dimensions) and the energy equation (conservation of heat). They describe the flow variables: both the velocities \(u\) and \(v\), the pressure \(p\) and the temperature \(T\) as a function of the independent variables \(x, y\) and \(t\). In literature, e.g. [7], these equations can be found. To apply these equations, it is useful to make them dimensionless. This can be achieved by scaling the dependent and independent variables with meaningful reference quantities.

In this situation, it is straightforward to use the height \(H\) as the reference quantity for the coordinates in the \((x, y)\)-plane. The height-to-width aspect ratio \((A_y)\) and the depth-to-width ratio \((A_z)\) could formally affect the flow character through the boundary conditions [4,8], but they are (relatively) close to unity for our set-up. We use a width-to-height ratio \(W/H = 1/2\).

The temperature is scaled by the mean temperature \(T_{\text{ref}}\) and by the temperature difference \(\Delta T\), because both are characteristics of the cavity. No direct reference velocity is available. Henkes [9] shows that for the flows in this study, the Brunt-Väisälä velocity scale, defined as:

\[
\upsilon_{BV} = \sqrt{gH\beta_T \Delta T}
\]  

(3.1)
is an appropriate reference velocity. With this reference velocity, we can scale time by using \(H/\upsilon_{BV}\) as reference time and \(\rho \upsilon_{BV}^2\) as reference pressure. We can combine these reference quantities, to scale the variables as follows:

\[
X_D = \frac{x}{H}
\]  

(3.2)
40 \hspace{1cm} \textit{CHAPTER 3. TEMPERATURE-DRIVEN NATURAL CONVECTION}

\begin{align*}
y_D &= \frac{y}{H} \hspace{1cm} (3.3) \\
t_D &= \frac{t_{uv}}{H} \hspace{1cm} (3.4) \\
p_D &= \frac{P}{\rho u_{BV}^2} \hspace{1cm} (3.5) \\
T_D &= \frac{T - T_{ref}}{\Delta T} \hspace{1cm} (3.6) \\
u_D &= \frac{u}{u_{BV}} \hspace{1cm} (3.7) \\
v_D &= \frac{v}{u_{BV}} \hspace{1cm} (3.8)
\end{align*}

Using these scale relations, Eqs. 3.2 to 3.8, we can write the Boussinesq equations for continuity, momentum, and energy as:

\begin{align*}
\frac{\partial u_D}{\partial x_D} + \frac{\partial v_D}{\partial y_D} &= 0 \hspace{1cm} (3.9) \\
\frac{\partial u_D}{\partial t_D} + u_D \frac{\partial u_D}{\partial x_D} + v_D \frac{\partial u_D}{\partial y_D} &= -\frac{\partial p_D}{\partial x_D} + \sqrt{\frac{Pr}{Ra}} \left( \frac{\partial^2 u_D}{\partial x_D^2} + \frac{\partial^2 u_D}{\partial y_D^2} \right) - T_D \cos \theta \\
\frac{\partial v_D}{\partial t_D} + u_D \frac{\partial v_D}{\partial x_D} + v_D \frac{\partial v_D}{\partial y_D} &= -\frac{\partial p_D}{\partial y_D} + \sqrt{\frac{Pr}{Ra}} \left( \frac{\partial^2 v_D}{\partial x_D^2} + \frac{\partial^2 v_D}{\partial y_D^2} \right) - T_D \sin \theta \hspace{1cm} (3.10) \\
\frac{\partial T_D}{\partial t_D} + u_D \frac{\partial T_D}{\partial x_D} + v_D \frac{\partial T_D}{\partial y_D} &= \sqrt{\frac{1}{RaPr}} \left( \frac{\partial^2 T_D}{\partial x_D^2} + \frac{\partial^2 T_D}{\partial y_D^2} \right) \hspace{1cm} (3.11)
\end{align*}

where $\theta$ is the inclination angle, defined as the angle between the top and the gravity vector.

The boundary conditions are given by (using $W/H = 1/2$):

\begin{align*}
T_D(x_D = 0, 0 < y_D < 1) &= \frac{1}{2}, \\
T_D(x_D = 1/2, 0 < y_D < 1) &= \frac{1}{2}, \\
\int_0^{1/2} q(x_D, y_D = 0) dx &= 0, T_D(x_D, y_D = 0) = \text{constant}_1, \\
\int_0^{1/2} q(x_D, y_D = 1) dx &= 0, T_D(x_D, y_D = 1) = \text{constant}_2.
\end{align*}
Constant_1 and constant_2 appear in the last two boundary conditions because the top and bottom temperatures are allowed to equilibrate, i.e., are neither heated nor cooled. In our set-up this leads to a constant temperature distribution along the top- and bottom-plates which is higher near the (hot) left wall and lower near the (cold) right wall. The temperature difference along the plates is approximately 5 degrees Kelvin. Equations 3.9, 3.10, 3.11, and 3.12 show that flow is can be described by only two dimensionless numbers, the Prandtl number:

\[ Pr = \frac{\mu C_p}{\lambda} \tag{3.13} \]

and the Rayleigh number:

\[ Ra = \frac{g \rho^2 \beta T \Delta T H^3}{\mu^2} Pr \tag{3.14} \]

Under our experimental conditions the values for \( Pr \) and \( Ra \) are 0.71 and \( 5 \cdot 10^9 \), respectively. We also define the ratio \( W/H \) as a dimensionless number, but, since the width of the boundary layer width is much smaller than the distance between the side walls we assume that its influence can be neglected. The physical significance of the Prandtl number is the ratio between the temperature boundary layer and the velocity boundary layer thickness. Flow is fully described by the Rayleigh number, together with the temperatures of the top and bottom. The Rayleigh number is the ratio between the buoyancy forces and the viscous forces. If the Rayleigh number is high, buoyancy forces dominate and flow will be turbulent. At our Rayleigh number, flow in a rectangular enclosure which has adiabatic top and bottom is still in transition from the laminar to the turbulent regime. We will see that since the top and bottom of the rectangular convection chamber used are isothermal rather than adiabatic, a value of \( 5 \cdot 10^9 \) for the Rayleigh number results in well-developed, turbulent boundary layers. This observation was also made by Henkes [9], on the basis a numerical study.

### 3.2.1 Turbulent natural convection

Turbulent fluctuations of the variables are described by means of statistical methods. The simplest way to do this in a steady flow is by applying the Reynolds decomposition (for details, see e.g. Tennekes and Lumley [10]), in which we write a variable \( \varphi \) as the sum of a time-independent expected mean value \( \bar{\varphi} \), and a time-dependent fluctuating value \( \varphi' \):

\[ \varphi(t) = \bar{\varphi} + \varphi'(t) \tag{3.15} \]

If the Reynolds decomposition is applied to the Boussinesq equations 3.10, 3.11, and 3.12, new terms containing the fluctuations are introduced: \( -\rho u_i' u_j' \) and \( -\rho u_i' T' \). Both terms are unknowns, which makes the number of unknowns larger than the number of equations. Therefore, additional relations are required.
to reach a solution. These additional relations are often called the turbulence-closure relations.

The term \(-\rho u'_i u'_j\) can be viewed as the turbulent transport in the \(j\)-direction of the momentum in the \(i\)-direction. This momentum transport bears some analogy to tension acting on a surface, and for that reason it is called the Reynolds stress. In a similar way, the term \(-\rho u'_i T'\) can be regarded as the turbulent heat flux, or Reynolds flux, resulting from velocity fluctuations. A model for solving the closure problem introduces an eddy-viscosity \(\mu_t\). Analogous to the linear relationship between the deviatoric stress and the deformation tensor, the following relations can be written for the \(j\)-th component of the Reynolds stresses and fluxes:

\[
\rho \left( u'_i u'_j + \frac{1}{3} k \delta_{ij} \right) = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{3.16}
\]

\[-\rho u'_i T' = \frac{\mu_t}{\sigma_t} \frac{\partial T'}{\partial x_i} \tag{3.17}\]

here \(\sigma_t\) is the turbulent Prandtl-number which equals one for most turbulent flows, according to Hinze [11], and \(k\) is the turbulent kinetic energy:

\[
k = \frac{1}{2} \sum_{i=1}^{3} u'_i u'_i \tag{3.18}\]

The relations above model the Reynolds stress and the turbulent heat flux by velocity fluctuations, but still leave two unknowns. Several so-called turbulence models have been developed to solve this problem. The turbulence models used in this study consider \(\mu_t\) to be a function of \(k\) and \(\epsilon\), the turbulent kinetic energy and its dissipation (for details, see e.g. Launder and Spalding [12] or Mohammadi [13]). These turbulence models contain empirical constants. In the simulations of this study, the conventional standard \(k - \epsilon\)-model [6,14], and the low-Reynolds number \(k - \epsilon\) model, developed by Chien [15] are used.

### 3.3 Laser Doppler anemometry

#### 3.3.1 Measurement of particle velocities using the Doppler effect

In this study, we have used laser Doppler anemometry (LDA) to measure velocity fields in the experimental set-ups described later in this chapter. Details of the LDA technique itself can be found in standard textbooks [16,17]. Here, we give a brief discussion of the main principles of LDA, and highlight specific aspects of the set-up.
The advantages of the LDA-technique are clear: it is a non-intrusive, non-disturbing technique which enables measuring velocities in small volumes. Furthermore, temporal fluctuations of the flow can be determined because of the short measuring times. There are, however, some disadvantages to this technique: the flow has to be seeded with particles that can be detected, and the measuring points have to be accessible for optic beams.

The LDA technique is based on the fact that light, scattered from a moving particle has a shifted frequency (see Fig. 3.2). Light emitted from a stationary source is scattered towards a stationary observer by a moving particle. The observer sees light that has a shifted frequency as a result of the Doppler effect. The frequency shift or Doppler shift, \( f_d \), is determined by the velocity of the particle and the direction in which it moves relative to source and observer (see e.g. Durst [16]):

\[
f_d = f \frac{|\vec{u}|}{c} (\cos \beta + \cos \gamma)
\]  

in which \( c \) is the velocity of light, \(|\vec{u}|\) is the magnitude of the velocity of the moving particle, \( \beta \) is the angle between the emitting source and the direction of the moving particle, and \( \gamma \) is the angle between the observer and the moving particle.

### 3.3.2 The Differential Doppler Anemometer

The optical configuration that we used for the differential Doppler measurements is shown in Fig. 3.3. A 4-Watt Argon-ion laser produces a beam which is split in two. One of these two beams passes through a Bragg-cell and is preshifted in frequency. This preshift, enables discrimination of the flow direction in the
convection chamber can be discriminated. The other beam passes through a glass rod to make up for the difference in path length caused by the Bragg cell. Both beams are split into a blue (488 nm) and a green (514.5 nm) beam. Each of the four beams is transported to the probe through a separate fibre-optic cable. In the laser probe, all the optics for proper alignment are present. The beam separation is 38 mm, and the beam diameters are 1.35 mm. A beam expander enhances the beam separation to 73.7 mm, and with a 310 mm front lens, this results in a measurement volume which is 0.63 mm long and 75 μm in diameter. Scattered light from either smoke or specially treated Al₂O₃ seeding particles moving through the measurement volume is focussed on a fifth fibre-optic cable. The scattered light passes through a colour separator, and photo multipliers transform the optical signal into an electrical signal.

**Signal Processing**

The principle of signal processing for one signal (green or blue) is presented in Fig. 3.4. A down mixer reduces the optical preshift of 40 MHz to the desired frequency range, usually 150 kHz. A bandpass filter cuts off low-frequency pedestal and high-frequency noise. The filtered signals are monitored on an oscilloscope for on-line and real-time visual feedback and quality control. The signal analysis is performed by two TSI Intelligent Flow Analysers (IFA) 550 [18]. The
Doppler frequency is measured by timing eight successive zero-crossings. The resulting zero-crossing pulses are then checked by a validation algorithm to determine whether the zero-crossings were produced by a coherent signal or by noise. An estimate of the expected frequency is required by this algorithm. After being detected by an IFA, the validated burst is read and stored by a software controlled interface board on a PC. Both interface board and software have been developed at the Section Heat Transfer of the Faculty of Applied Physics of Delft University of Technology.

3.4 Rectangular Convection Chamber

A schematic representation of the convection chamber is shown in Fig. 3.1. The dimensions of the chamber $H \times W \times D$ are $0.95 \times 0.48 \times 0.49 \text{ m}^3$. The entire convection chamber can be placed at an angle $\theta$ between the negative $x$-axis and the gravitation vector $g$. The enclosed convection chamber consists of four 5 mm thick copper top, bottom, and side-wall plates. Temperatures of all four walls are monitored during measurements by 32 copper-constantan thermocouples, 11 on each of the vertical walls, and 5 on each of the horizontal walls. A high-resolution image of the temperature distribution on the walls is measured with an infrared camera. The wall temperatures were needed as boundary conditions for the numerical simulations to validate the measurements [5,6,19]. The hot wall is heated to an average temperature, $T_h$, of 343 K by circulating hot water from a constant-temperature bath through heating elements on the outside of the wall. The cold wall is cooled to an average temperature, $T_c$, of 293 K by circulating cold water from a constant-temperature bath through cooling elements on the outside of the wall. Through the top and bottom plates water is circulating which is neither heated nor cooled in order to obtain a constant temperature distribution.
Table 3.1: Average wall temperatures.

<table>
<thead>
<tr>
<th>Location</th>
<th>Temperature [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Left wall (hot)</td>
<td>355.2</td>
</tr>
<tr>
<td>Right wall (cold)</td>
<td>301.2</td>
</tr>
<tr>
<td>Top</td>
<td>328.2</td>
</tr>
<tr>
<td>Bottom</td>
<td>323.2</td>
</tr>
</tbody>
</table>

at these walls. All walls are insulated with 20 mm thick poly-urethane foam panels on the outside in order to minimize heat loss to the surroundings. The front and rear walls are made of 5 mm thick poly-carbonate plates which are insulated with 20 mm thick poly-urethane foam panels. Slots in the poly-urethane foam in the front wall enable laser light to enter the chamber and scattered light to leave the chamber.

3.4.1 Results obtained with the rectangular convection chamber

In this section, we focus on the influence that an inclination with the horizontal of the differentially heated convection chamber has on the flow structure. Since a two-dimensional LDA device was used, only the average velocities and velocity fluctuations in the $x$ and $y$ direction were measured. This makes it impossible to use Eq. 3.18 directly. Instead we use a relationship obtained by Peeters and Henkes [20] from a numerical study:

$$k_{P\&H} = 3/4 \left( \overline{u'^2} + \overline{v'^2} \right)$$  \hspace{1cm} (3.20)

An experimental validation of this relationship is given in Appendix 3A. We performed velocity and turbulence measurements placing the convection chamber under three different angles with the horizontal: 90, 75, and 58 degrees. The hot wall is the lower (left) wall in the inclined situation. Each of the velocity and turbulent kinetic energy profiles presented in one figure contains profiles along the same line in the cavity under the three different angles of inclination (90, 75, and 58 degrees with the horizontal). Figure 3.5 shows the profiles along which the measurements were taken. Also depicted are the positions of the tilted convection chamber. All measurements were taken at half the chamber depth: $z = D/2 = 0.245$ m. Table 3.1 lists the average left wall (hot), right wall (cold), top, and bottom temperature. To characterize the shape of the velocity profiles and the turbulent kinetic energy profiles, eighteen measuring points were taken per line. These points are distributed in such a way that the boundary layers, in which the largest gradients appear, contain more measuring points than the stratified centre of the cavity. To get an indication of the flow in the
Figure 3.5: Horizontal and vertical measurement profile locations, at heights \(H/4, H/2, 3H/4\), and widths \(W/4, W/2, 3W/4\), respectively, are shown in dashed lines for the chamber in vertical position \((\theta = 90^\circ)\). All profiles were measured at half the chamber depth, \(D/2\). The positions of the tilted chamber with identical profile locations are shown by the dotted lines.

entire convection chamber, we measured profiles both parallel and perpendicular to the left (hot) wall. A general observation is that the width of both the hot wall boundary layer and the cold wall boundary layer increase at a decreasing inclination angle. This can be observed for the velocity as well as for the turbulent kinetic energy.

The profiles of the vertical velocity of Fig. 3.6a, 3.6b, and 3.6c show boundary layer behaviour along the hot and the cold wall. The width of these boundary layers increases when the angle of inclination decreases. The maximum velocity in the boundary layer is of the same order of magnitude and has approximately the same position for all three angles. This indicates that more mass is circulating in the inclined situation. An increasing instability in an inclined cavity towards a situation in which heating from below occurs, is the most probable cause.

In the horizontal velocity profiles at a vertical line of Fig. 3.7a, 3.7b, and 3.7c boundary layer structures are noticed as well. No measurements of horizontal velocity profiles have been performed at an inclination angle of 90\(^\circ\) at the tabulated boundary conditions, because of experimental problems. The boundary layers along the top and bottom are still developing at the first encountered profile: \(x = W/4 = 0.12\) m for the top boundary layer and \(x = 3W/4 = 0.36\) m for
the bottom boundary layer.

The profiles of the turbulent kinetic energy in Fig. 3.8a, b, and c show that the flow contains turbulent velocity fluctuations. The intensity of the turbulence can be defined as $\sqrt{\nu^2}/u$, in which $u$ is the velocity in the direction of the main flow. In the boundary layer, turbulence intensity is over 20%.

The turbulent kinetic energy develops along the hot and cold wall. At $y = 3H/4 = 0.72$ m, the turbulent kinetic energy is larger at the hot wall than at the cold wall, as shown in Fig. 3.8a. In the profile at half the cavity height, $y = H/2 = 0.48$ m, the turbulent kinetic energies at both walls are approximately equal, Fig. 3.8b.

The vertical profiles of the turbulent kinetic energy show that the turbulent kinetic energy in the top boundary layer and in the bottom boundary layer is smaller than in the boundary layers along the hot and the cold wall. At $y = H/4 = 0.24$ m, the turbulent kinetic energy is much smaller at the hot wall than at the cold wall, as is shown in Fig. 3.8c. In Fig. 3.9a, the profile at $x = W/4 = 0.12$ m was measured close to the boundary layer along the hot wall, and in Fig. 3.9c the profile at $x = 3W/4 = 0.36$ m is located close to the boundary layer along the cold wall. Therefore, the turbulent kinetic energy will not be zero on this profile. The profile shown in Fig. 3.9b at $x = W/2 = 0.24$ m has lower minimum values of the turbulent kinetic energy. In contrast with the 75° case, the turbulent kinetic energy is not close to zero for the inclination angle of 58°. This might be a result of a three-dimensional effect. In the profile at $x = W/2 = 0.24$, a boundary-layer structure can be observed.
Figure 3.6: Vertical velocity profiles at three horizontal lines: $y = H/4 = 0.24$ m, $y = H/2 = 0.48$ m, and $y = 3H/4 = 0.72$ m with inclination angles of $58^\circ$ (□), $75^\circ$ (+), and $90^\circ$ (∞). Table 3.1 lists the average wall temperatures.
Figure 3.7: Horizontal velocity profile at three vertical lines: $x = W/4 = 0.12$ m, $x = W/2 = 0.24$ m, and $x = 3W/4 = 0.36$ m with inclination angles of 58° (□), and 75° (++) . Table 3.1 lists the average wall temperatures.
3.4. RECTANGULAR CONVECTION CHAMBER

Figure 3.8: Profiles of the turbulent kinetic energy at three horizontal lines: $y = H/4 = 0.24$ m, $y = H/2 = 0.48$ m, $y = 3H/4 = 0.72$ m at inclination angles of $58^\circ$ (square), $75^\circ$ (plus), and $90^\circ$ (circle). The average wall temperatures are listed in Table 3.1.
Figure 3.9: Profiles of the turbulent kinetic energy at three vertical lines: 
\(x = W/4 = 0.12 \text{ m}, x = W/2 = 0.24 \text{ m}, \text{ and } x = 3W/4 = 0.36 \text{ m},\) 
with inclination angles of 58° (- - -), and 75° (- - -). The average wall temperatures are listed in Table 3.1.
3.5 Measurements vs. numerical calculations

For a numerical simulation of a natural-convection flow, several turbulence models have been developed. To determine which turbulence model provides the best match with the measured data, we have simulated the measurements with the standard $k - \epsilon$ model, and with a low Reynolds-number $k - \epsilon$ model, developed by Chien [15]. The most important and remarkable differences and similarities are discussed.

In the vertical velocity profiles of Fig. 3.10a, the measurements and the simulations using the Chien model show good agreement. The simulated velocities at vertical profiles, calculated with the standard $k - \epsilon$ and with the Chien model, matches the velocity profiles parallel to the hot and the cold walls very well. An example is given in Fig. 3.11a. Again, it can be noted that the calculations using the Chien simulations provide a better match.

The calculated profiles of the turbulent kinetic energy also resemble the results of the measurements. The width of the boundary layers calculated using the Chien turbulence model is smaller than the width of the boundary layer calculated with the standard $k-\epsilon$ model. In general, it is observed that the Chien turbulence model matches the measurements better than the $k-\epsilon$ model.

Example of a horizontal velocity profile and for a vertical turbulent kinetic energy profile are given in Fig. 3.10b and Fig. 3.11b. Here, simulations and measurements match generally well for the average velocities in Fig. 3.10b, but show some difference in the centre of the chamber for the turbulent kinetic energy profile. The fact, that here measured turbulent kinetic energies are higher than the simulated ones, can possibly be attributed to a three-dimensional effect.

The averaged Nusselt numbers resulting from the numerical calculations at the three different angles increases for a decreasing angle, which is in agreement with the observation that more mass is circulating at lower inclination angles. A similar observation was made by Kuyper [3] in a numerical study of turbulent flows in square, differentially heated enclosures.

The asymmetry in the turbulent kinetic energy in the boundary along the hot and cold wall layers in the profiles at $y = H/4 = 0.24$ m $y = 3H/4 = 0.72$ m is predicted well by the simulations, as can be seen in Fig. 3.12. Here the Chien model again gives a better match than the standard $k - \epsilon$ model.
Figure 3.10: Vertical velocity and turbulent kinetic energy profiles at a horizontal line $y = H/2 = 0.48$ m, $\theta = 90^\circ$, measured (□) and simulated both with the standard $k - \epsilon$ model (---) and the Chien model (---). The average wall temperatures are listed in Table 3.1.
Figure 3.11: Horizontal velocity and turbulent kinetic energy profiles at a vertical line $x = W/2 = 0.24$ m, $\theta = 58^\circ$, measured (□) and simulated both with the standard $k - \epsilon$ model (-) and the Chien model (--). The average wall temperatures are listed in Table 3.1.
Figure 3.12: Horizontal profiles of the turbulent kinetic energy, measured (□) and simulated both with the standard $k - \varepsilon$ model (---) and the Chien model ( - - ). The average wall temperatures are listed in Table 3.1. a: $y = 3H/4 = 0.72$ m, $\theta = 58^\circ$; b: $y = H/4 = 0.24$ m, $\theta = 75^\circ$.

3.6 Conclusions

- The flow shows a typical boundary-layer behaviour for all three angles of inclination. The width of the boundary layers along the two sidewalls was found to increase for a low angle of inclination, whereas the maximum velocity remained virtually unchanged. This means that at low angles,
more mass is circulating, indicating a higher heat transfer. The Nusselt numbers obtained from the numerical calculations confirm this trend.

- Our measurements validate the turbulence modelling that Kuyper used for his numerical studies of the underground coal gasification process. Measurements and numerical calculations are in close agreement, a low Reynolds turbulence model gives the best results for most of the cases observed.

3.7 Nomenclature

Latin
- \( c = \) velocity of light, \( \text{L} / \text{t}, \text{m} / \text{s} \)
- \( D = \) depth of the rectangular convection chamber, \( \text{L}, \text{m} \)
- \( f = \) frequency, \( 1 / \text{t}, 1 / \text{s} \)
- \( g = \) gravitation vector, \( \text{L} / \text{t}^2, \text{m} / \text{s}^2 \)
- \( H = \) height of the rectangular convection chamber, \( \text{L}, \text{m} \)
- \( k = \) turbulent kinetic energy, \( \text{L}^2 / \text{t}^2, \text{m}^2 / \text{s}^2 \)
- \( Nu = \) Nusselt number
- \( Pr = \) Prandtl number
- \( Ra = \) Rayleigh number
- \( T = \) Temperature, \( \text{T}, \text{K} \)
- \( u = \) horizontal velocity component, \( (u = \overline{u} + u'), \text{L} / \text{t}, \text{m} / \text{s} \)
- \( v = \) vertical velocity component, \( (v = \overline{v} + v'), \text{L} / \text{t}, \text{m} / \text{s} \)
- \( w = \) transverse velocity component, \( (w = \overline{w} + w'), \text{L} / \text{t}, \text{m} / \text{s} \)
- \( W = \) width of the rectangular convection chamber, \( \text{L}, \text{m} \)
- \( x = \) horizontal coordinate (positive in direction of \( u \))
- \( y = \) vertical coordinate (positive in direction of \( v \))
- \( z = \) transverse coordinate (positive in direction of \( w \))

Greek
- \( \beta = \) angle between direction of moving particle and source, \( ^\circ \)
- \( \beta_T = \) thermal expansion coefficient, \( 1 / \text{T}, 1 / \text{K} \)
- \( \delta_{ij} = \) Kronecker delta
- \( \epsilon = \) dissipation rate of turbulent kinetic energy, \( \text{L}^2 / \text{t}^2, \text{m}^2 / \text{s}^2 \)
- \( \mu = \) dynamic viscosity, \( \text{m} / \text{Lt}, \text{Pa.s} \)
- \( \rho = \) density, \( \text{m} / \text{L}^3, \text{kg} / \text{m}^3 \)
- \( \sigma = \) turbulent Prandtl number
- \( \theta = \) angle with respect to the horizontal, \( ^\circ \)

Subscripts
- \( BV = \) Brunt-Väisälä
c = cold

d = Doppler

D = dimensionless

est = estimated

h = hot

i, j = coordinate index

m = measured

P&H = Peeters & Henkes

t = turbulent
Bibliography


Appendix 3A

Turbulent kinetic energy

3A.1 Introduction

In this appendix a relationship is presented to derive the turbulent kinetic energy directly from fluctuations of only two velocity components. The relationship is compared both with a numerical relationship and a direct determination from fluctuations of all three velocity components.

Wall-bounded turbulent flows usually show strong anisotropy. Velocity fluctuations in the main-flow direction can develop freely, whereas velocity fluctuations perpendicular to the bounding wall are damped. Velocity fluctuations in the third dimension receive energy from the main flow by velocity-pressure gradient correlations [21] and are not damped. Turbulence statistics have been studied extensively for forced-convection (shear-driven) channel flows. An overview of the work on these flows has been given by Kim et al. [22]. Direct numerical simulation [23, 24] and three-dimensional measurements [25] have revealed the anisotropy of shear-driven turbulent boundary layers. The available data were applied to improve Reynolds-stress models and, consequently, most of the available turbulence models were derived for forced-convection flow.

Tsuiji and Nagano [26, 27] showed that some characteristics of buoyancy-driven turbulent boundary layers differ significantly from shear-driven boundary layers. Since numerical simulations of these flows are often performed by using $k$-$\varepsilon$ models [28], it is interesting to validate the assumed isotropy in these models. Peeters and Henkes [20] applied Reynolds-stress models to simulate the turbulent boundary layer along a heated plate and obtained a prediction for the fluctuations in all three dimensions.

3A.2 Results

In Fig. 3A.1a results for the average horizontal and vertical velocity ($\bar{u}$ and $\bar{v}$, respectively) at half the rectangular enclosure height ($y = H/2$) are presented.
The plot for $\overline{v}$ shows that the maximum velocity along the hot wall is higher than the maximum velocity along the cold wall, whereas the hot-wall boundary layer is smaller than the cold-wall boundary layer. This difference is probably due to the slightly non-symmetrical temperatures of the horizontal walls and the difference in the fluid density at the hot and cold wall. The horizontal velocities at half the enclosure height are small. In Fig. 3A.1b the root-mean-square of the velocity fluctuations in the $x$- and $y$-direction are presented as a function of the distance from the hot wall. The fluctuations in the hot- and cold-wall boundary layer are remarkably similar, although the cold-wall boundary layer is slightly wider than the hot-wall boundary layer. The kinetic energy of the fluctuations in the horizontal direction is considerably smaller than in the vertical direction as a result of damping by the bounding walls. Halfway between the isothermal walls, both fluctuating components give rise to equal kinetic energies, which shows the isotropy of turbulence in the centre of the enclosure. If the experimental results have to be used to validate numerical simulations in which an equation for $k$ is solved instead of equations for all velocity fluctuations, it is necessary to combine the results for $\sqrt{u'^2}$ and $\sqrt{v'^2}$ to build up a value for $k$. Since, by definition,

$$k = 1/2 \left( u'^2 + v'^2 + w'^2 \right)$$

a value for $k$ can be derived by either

1. measuring $u'^2$, $v'^2$ and $w'^2$ or

2. measuring $u'^2$ and $v'^2$ and calculating $w'^2$ from these values.

In this appendix, option 1 is applied on a few points. The observed relationship between $u'^2$, $v'^2$, and $w'^2$ is used to obtain a value of $k$ by option 2 on points where only $u'^2$ and $v'^2$ have been measured.

It is necessary to rotate the two-dimensional measuring probe under three different angles $\phi$ in order to obtain the $w$-component of the flow inside the convection chamber. This is illustrated by Fig. 3A.2. For this study, measurements were taken from a point located at 0.015 m distance from the hot wall. This point is in the high velocity area of the (turbulent) boundary layer, beyond the maximum. The probe was rotated under $15^\circ$, $30^\circ$, and $45^\circ$ angles. The measured velocity can be decomposed in the two velocity components in the horizontal plane, $u$ and $w$ (see Fig. 3A.2), by

$$u_m = u \cos \phi + w \sin \phi$$  \hspace{1cm} (3A.1)

in which the subscript $m$ denotes the measured velocity. This relationship is also valid for the average velocity. When the average velocity is measured at two known angles with the vertical wall, the average value of $u$ and $w$ can be deduced.
3A.2. RESULTS

**Figure 3A.1:** Average velocity profiles and velocity fluctuations at $y = \frac{H}{2} = 0.48$ m. $\theta = 90^\circ$. 
The fluctuations of $u$ and $w$ can also be deduced from these measurements. When the Reynolds-decomposition is applied, Eq. (3A.1) can be written as

$$
\overline{u_m} + u'_m = (\overline{u} + u') \cos \phi + (\overline{w} + w') \sin \phi
$$

(3A.2)

From Equation (3A.2), the average velocity is subtracted. The remaining equation is squared and averaged, leading to:

$$
\overline{u'_m^2} = \overline{u'^2} \cos^2 \phi + \overline{w'^2} \sin^2 \phi + 2\overline{u'w'} \sin \phi \cos \phi
$$

(3A.3)

This relationship contains three unknowns, the desired $\overline{u'^2}$ and $\overline{w'^2}$, and a Reynolds-stress term $\overline{u'w'}$. By measuring the velocity under three different angles, the velocity components $u$, $v$, $w$, and their turbulent fluctuations can be calculated.

The results of the measurements in which the probe is rotated are presented in Table 3A.1. At five different heights in the convection chamber close to the top, the average velocity and the velocity fluctuations are determined. The average velocity in the vertical direction is high and decreases slightly with increasing height, as a result of the vicinity of the top. Both $\overline{u}$ and $\overline{v}$ are small. The fluctuations in the vertical direction are stronger than in the other directions and contribute largely to the turbulent kinetic energy. Except for one point ($y = 0.74$ m), at all points we have $\sqrt{\overline{u'^2}} < \sqrt{\overline{w'^2}} < \sqrt{\overline{v'^2}}$. A good estimation of $\sqrt{\overline{w'^2}}$ from $\sqrt{\overline{u'^2}}$ and
Table 3A.1: Velocity components \( u, v, \) and \( w, \) turbulent velocity fluctuations and turbulent kinetic energies (\( \overline{k} \) calculated from 3D data and \( k_{\text{est}} \) calculated from \( u \) and \( v \) data only, using Eq. 3A.4), at five different heights in the convection chamber, at 0.015 m distance from the hot wall.

<table>
<thead>
<tr>
<th>property</th>
<th>dimension</th>
<th>( y ) [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.72</td>
</tr>
<tr>
<td>( \overline{u} )</td>
<td>[m/s]</td>
<td>-0.0102</td>
</tr>
<tr>
<td>( \overline{v} )</td>
<td>[m/s]</td>
<td>0.1839</td>
</tr>
<tr>
<td>( \overline{w} )</td>
<td>[m/s]</td>
<td>0.0015</td>
</tr>
<tr>
<td>( \sqrt{\overline{u'^2}} )</td>
<td>[m/s]</td>
<td>0.0403</td>
</tr>
<tr>
<td>( \sqrt{\overline{v'^2}} )</td>
<td>[m/s]</td>
<td>0.0548</td>
</tr>
<tr>
<td>( \sqrt{\overline{w'^2}} )</td>
<td>[m/s]</td>
<td>0.0479</td>
</tr>
<tr>
<td>( k )</td>
<td>[m²/s²]</td>
<td>0.0035</td>
</tr>
<tr>
<td>( k_{\text{est}} )</td>
<td>[m²/s²]</td>
<td>0.0035</td>
</tr>
<tr>
<td>Deviation</td>
<td>[%]</td>
<td>0.0</td>
</tr>
</tbody>
</table>

\( \sqrt{\overline{v'^2}} \) is obtained by using

\[
\overline{v'^2} = \frac{\overline{u'^2} + \overline{v'^2}}{2}, \quad \text{so} \quad k_{\text{est}} = \frac{3}{4} \left( \overline{u'^2} + \overline{v'^2} \right)
\]

(3A.4)

This estimation is in good agreement with a relationship presented by Peeters and Henkes [20] from a numerical study. The measured \( k \) and the value of \( k \) estimated from \( \overline{u'^2} \) and \( \overline{v'^2} \) by Eq. 3A.4 are added in Table 3A.1. The turbulent kinetic energies derived from the fluctuations of all three velocity components are in good agreement with turbulent kinetic energies calculated using only \( \overline{u'^2} \) and \( \overline{v'^2} \). With this observation, we can now calculate the turbulent kinetic energy profiles from our two-dimensional measured data. Throughout the chapter this relationship was used to determine the turbulent kinetic energy profiles (Figs 3.8 and 3.9). In Figs 3.10b, 3.11b, and 3.12b profiles of \( k_{\text{est}}, \) (or \( k_{P&H} \)) are compared with numerical-simulation results.

### 3A.3 Conclusions

From the results presented in this appendix, we can draw the following conclusions. The measurement of the three velocity components and their fluctuations
in a two-dimensional LDA system require that the probe is rotated under three
different angles. Results of the measurements show the relative magnitude of
the velocity fluctuations in buoyancy-driven turbulent boundary layers. Fluctua-
tions in the main-flow direction are strongest, fluctuations perpendicular to the
bounding wall are weakest. The kinetic energy of the fluctuations in the third
dimension can be estimated by using the mean value of the kinetic energy of the
fluctuations in the other directions. By using $k_{est} = 3/4 \left( \bar{u}^2 + \bar{v}^2 \right)$ we can now
deduce a turbulent kinetic energy from two-dimensional measured data.
Chapter 4

Double-diffusive natural convection

In this chapter laser Doppler measurements in a trapezoidal differentially heated chamber, in which composition differences can also be introduced as driving force, in order to study double-diffusive natural convection flows. Temperature driven measurements are presented, as well as a visualisation of the flow pattern inside the enclosure. LDA measurements compare reasonably well with numerical results. A limited number of measurements of the double-diffusive situation is presented, in which temperature- and composition-driven natural convection flows are opposed.

4.1 Introduction

The framework for the double-diffusive natural convection studies is derived from the underground cavity that forms during the initial stages of underground coal gasification. A conceptual picture of the initial cavity development is shown in Fig. 4.1. It shows a cross-section of a gasification channel. After the very first gasification has taken place, a cavity is formed with ash at the bottom, covering the original injection channel. On top of the ash we find rubble which has spalled from the roof, and char spalled from the coal surface. Injected air enters the cavity from below. At the sides the air will react with the char and thus form CO. The air in the centre will react with the combustible gases present in the cavity to form CO₂. It is asserted that the hot CO₂ rises to the upper part of the cavity and deflects to the side roofs of coal to react endothermically (CO₂ + C → 2CO) [1,2].

The relatively cold CO descends and serves partly as a reaction agent for the injected air and is partly produced via the producing well (not shown in the figure). In summary the natural convection flows are double-diffusive, i.e., driven by the density variations as a result of heterogeneous temperature and composition distributions in the cavity.

There are few experimental data regarding double-diffusive natural convection in literature [3–6]. The main subject of these articles is laminar flow, whereas
Figure 4.1: A conceptual picture of initial gasification cavity development.

we emphasise turbulent flows. In this chapter, we present laser Doppler (LDA) and visualisation experiments on turbulent natural convection flows, and compare these measurements with results obtained from numerical models. The purpose of this study is to validate the numerical models which are used to calculate double-diffusive turbulent natural convection flow [2, 7]. Furthermore, the experimental results can pinpoint certain situations in which, in a typical underground coal gasification situation, the mass transfer is hampered by opposing driving forces.

4.2 The trapezoidal convection chamber

We have constructed a physical model in which double-diffusive flow can be studied. The model has the shape of a trapezoid the (inner) dimensions of which are: $H = 0.35$ m, $W = 0.96$ m, and $D = 0.51$ m. A schematic representation of this trapezoidal convection chamber is shown in Fig. 4.2. Each side of the trapezoidal set-up can be maintained at a specified temperature to induce natural convection flows. Furthermore, gases can be injected into the trapezoidal convection chamber, which makes the flow double diffusive.

This trapezoidal shape was chosen to simulate the shape of the initial developing stages of a gasifier as closely as technically possible. Indeed, after validation of the numerical models it is relatively simple to numerically simulate flows for other, more realistic, cavity shapes.

The insulated top plate is 0.25 m wide and 0.51 m deep. The resulting angle of the two side walls with the horizontal is 45 degrees. The two side walls and the bottom plates consist of copper segments (see Fig. 4.3) that can be either heated or cooled. Each of the plates has a special structure to facilitate simultaneous thermostating and gas injection. In the experimental model we use two different
gases: argon to represent CO$_2$ and nitrogen to represent CO.

The chamber's base plates are heated to an average temperature $T_h$ of 315 K by circulating hot oil from a constant-temperature bath through the eight heating elements. The side walls are cooled to an average temperature $T_c$ of 285 K by circulating cold water from a constant-temperature bath through the four cooling elements. Each thermostated plate has six locations where thermocouple measurements can be taken with Chromel Alumel thermocouples. A dense pattern of orifices (6700/m$^2$) enables a uniform injection distribution of gases at the required temperature through twelve thermostated elements. The top is made of 25 mm thick perspex to enable laser sheet flow visualisation experiments. All walls are insulated with 20 mm thick poly-urethane foam panels on the outside in order to minimize heat losses to the surroundings. The front wall is made of a 5 mm thick poly-carbonate plate which is insulated with a 10 mm thick poly-urethane foam panel. Slots were cut in the poly-urethane foam in the front wall to allow for laser light to enter the chamber and scattered light to leave the chamber. The rear wall is permeable to the injected gases.

4.3 Mathematical formulation

Analogous to Chapter 3, we can derive the 2D equations of motion for fluid flow following from the conservation of chemical species, energy, mass, and momentum (see also, e.g., Bird [8]). Here we will restrict ourselves to presenting the equations in a dimensionless form, and give the dimensionless parameters that arise, as well as the boundary conditions. For a detailed derivation of the system of equations, see Van der Eyden [7].

Applying the Boussinesq approximation, we linearize the density in terms of temperature and mass fraction: $\rho \rho_0 = 1 - \beta_T(T - T_{ref}) - \beta_\omega(\omega - \omega_{ref})$, with $\beta_T$
CHAPTER 4. DOUBLE-DIFFUSIVE NATURAL CONVECTION

Figure 4.3: Vertical cross-section of the trapezoidal setup with heating and cooling elements.

the thermal expansion coefficient, and \( \beta \) the expansion coefficient determined by the mass fraction of the two components.

The system of equations is made dimensionless using the cavity height \( H \) as a length scale, \( \frac{\mu}{\rho_{ref} H^2} \) as a time scale, \( \frac{\mu^2}{\rho_{ref} H^2} \) as a pressure scale, the temperature difference \( \Delta T \) between the hot base plate and the cold side walls as a temperature scale, and the cold wall temperature as the reference temperature.

\[
\frac{\partial u_D}{\partial x_D} + \frac{\partial v_D}{\partial y_D} = 0
\]  
(4.1)

\[
\frac{\partial u_D}{\partial t_D} + u_D \frac{\partial u_D}{\partial x_D} + v_D \frac{\partial u_D}{\partial y_D} = -\frac{\partial p_D}{\partial x_D} + \left( \frac{\partial^2 u_D}{\partial x_D^2} + \frac{\partial^2 u_D}{\partial y_D^2} \right)
\]  
(4.2)

\[
\frac{\partial v_D}{\partial t_D} + u_D \frac{\partial v_D}{\partial x_D} + v_D \frac{\partial v_D}{\partial y_D} = -\frac{\partial p_D}{\partial y_D} + \left( \frac{\partial^2 v_D}{\partial x_D^2} + \frac{\partial^2 v_D}{\partial y_D^2} \right) + (Gr_T T_D + Gr_\omega \omega_D)
\]  
(4.3)

\[
\frac{\partial T_D}{\partial t_D} + u_D \frac{\partial T_D}{\partial x_D} + v_D \frac{\partial T_D}{\partial y_D} = \frac{1}{Pr} \left( \frac{\partial^2 T_D}{\partial x_D^2} + \frac{\partial^2 T_D}{\partial y_D^2} \right)
\]  
(4.4)
Table 4.1: Boundary conditions.

<table>
<thead>
<tr>
<th>Condition</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>bottom</td>
<td>$u_n = \frac{S_{h_{\text{heavy}}}}{Sc}$</td>
</tr>
<tr>
<td>left/right walls</td>
<td>$u_n = \frac{S_{h_{\text{light}}}}{Sc}$</td>
</tr>
<tr>
<td>top</td>
<td>$u_n = 0$</td>
</tr>
</tbody>
</table>

\[
\frac{\partial \omega_D}{\partial t_D} + u_D \frac{\partial \omega_D}{\partial x_D} + v_D \frac{\partial \omega_D}{\partial y_D} = \frac{1}{Sc} \left( \frac{\partial^2 \omega_D}{\partial x_D^2} + \frac{\partial^2 \omega_D}{\partial y_D^2} \right) \tag{4.5}
\]

The flow characteristics are determined by four dimensionless parameters:

\[
Gr_T = \frac{g \rho^2 \beta_T \Delta T H^3}{\mu^2} \quad \frac{\text{thermal buoyancy forces}}{\text{viscous forces}} \tag{4.6}
\]

\[
Gr_\omega = \frac{g \rho^2 \beta_\omega H^3}{\mu^2} \quad \frac{\text{solutal buoyancy forces}}{\text{viscous forces}} \tag{4.7}
\]

\[
Pr = \frac{\mu c_p}{\lambda} \quad \frac{\text{momentum diffusion}}{\text{thermal diffusion}} \tag{4.8}
\]

\[
Sc = \frac{\mu}{\rho D} \quad \frac{\text{momentum diffusion}}{\text{solutal diffusion}} \tag{4.9}
\]

The local mass transfer rates can be expressed by local Sherwood numbers, $S_{h_{\text{heavy}}}$ for the heavy gas, and $S_{h_{\text{light}}}$ for the light gas:

\[
S_{h_{\text{heavy}}} = \frac{\rho u_n \omega - \rho D \frac{\partial \omega}{\partial x_n}}{\rho D \frac{1}{H}} \tag{4.10}
\]

\[
S_{h_{\text{light}}} = \frac{\rho u_n (1 - \omega) + \rho D \frac{\partial \omega}{\partial x_n}}{\rho D \frac{1}{H}} \tag{4.11}
\]

in which $u_n$ is the velocity normal to the wall. These local Sherwood numbers can be considered equivalent to a Sherwood number that can be defined for underground coal gasification: $Sh = \frac{k H}{\rho D}$, with $k$ the mass-transfer coefficient.

The boundary conditions are listed in Table 4.1. The Sherwood numbers for the heavy and the light gas, together with the dimensionless Grashof, Prandtl, and Schmidt numbers, determine flow in the double-diffusive case.

### 4.4 Temperature-driven natural convection

#### 4.4.1 Visualisation experiments

The numerical simulation tools that are available to calculate double-diffusive natural convection flow are two-dimensional. If a comparison is to be made with
the LDA measurements, we have to make sure that the flow inside the convection chamber can be considered two-dimensional as well. To assess whether this is the case, we have performed several visualisation experiments in a temperature driven situation. The experiments make use of laser sheet visualisation. An extensive description of this technique can be found elsewhere, e.g. Opstelten [9]. The visualisation measurements were taken at two different cross-sections: one at \( W/2 \), and one at \( D/2 \), see Fig. 4.4.

Figure 4.5 shows a cross-section at half the cavity width (\( W/2 \)), perpendicular to the plane of the LDA measurements at \( D/2 \). The picture shows a single smoke plume rising to the cavity roof with no major deflections to the cavity's front or rear. This is an indication of the 2D nature of the flow inside the cavity. Figure 4.6 shows a smoke-visualisation picture with the illuminated plane at half the cavity depth (\( D/2 \)), in the plane of the LDA measurements. The left half of the cavity was illuminated during this experiment. The figure clearly shows the deflection of the smoke plume towards the cold side wall and from there downwards, indicated by an arrow.

## 4.4.2 LDA measurements

In this section we present LDA measurements in the trapezoidal convection chamber for temperature-driven natural convection, and compare the results with a low-Reynolds turbulence model [7]. For a description of the laser Doppler measuring technique, we refer to Chapter 3.

Figures 4.7, 4.8, and 4.9 show vertical and horizontal average velocity profiles measured and simulated at three different heights in the cavity. It should be noted that the rear wall was closed during velocity measurements, to increase residence time of the smoke particles, and thus increase effective LDA measuring-time. Table 4.2 lists the average wall temperatures during measurements. The velocity profiles were taken at three different heights: 0.37 \( H \), 0.54 \( H \), and 0.71 \( H \). The agreement between measurements and simulations ranges from fair to reasonable. In general, the match between the measured and simulated horizontal
Figure 4.5: Smoke visualisation experiment showing one single smoke plume rising to the cavity top with no major deflections to front or rear. The illuminated plane is located at $W/2$. The black arrows indicate the direction of flow, derived from the video recordings.

Figure 4.6: Smoke visualisation experiment showing a smoke plume along the upper part of the cold side wall, extending downward along the side wall. The illuminated plane is located at half the cavity depth ($D/2$). The black arrow indicates the direction of flow, derived from the video recordings.
velocity profiles is reasonable. The vertical velocity measurements show a slight asymmetry, which can be attributed to the slightly asymmetrical temperature distribution along the hot base plate. Furthermore, the calculated maximum central vertical velocity is higher than the measured maximum velocity for all profiles.

Figure 4.10 shows the near wall part of a turbulent kinetic energy profile measured at $y = 0.37 \mathcal{H}$ compared with a simulated profile. The agreement is reasonable for this (near-wall) part of the profile, but deteriorates further towards the middle of the chamber.

Figure 4.7: Horizontal and vertical velocity profiles, measured (+ vertical, and ◦ horizontal) and simulated with the low-Reynolds $k - \epsilon$ model (− vertical, and − horizontal). Profile at $y = 0.71 \mathcal{H}$. Table 4.2 lists the average wall temperatures.
Figure 4.8: Horizontal and vertical velocity profiles, measured (+ vertical, and ○ horizontal) and simulated with the low-Reynolds $k - \epsilon$ model (- - vertical, and – horizontal). Profile at $y = 0.54H$. Table 4.2 lists the average wall temperatures.

Figure 4.9: Horizontal and vertical velocity profiles, measured (+ vertical, and ○ horizontal) and simulated with the low-Reynolds $k - \epsilon$ model (- - vertical, and – horizontal). Profile at $y = 0.37H$. Table 4.2 lists the average wall temperatures.
$k_{P\&H}$

Figure 4.10: Turbulent kinetic energy profile $k_{P\&H}$, measured (○) and simulated (continuous line) with the low-Reynolds $k - \epsilon$ model. Profile taken near the left side wall at $y = 0.37H$. Table 4.2 lists the average wall temperatures.
4.5 Double diffusive natural convection

4.5.1 Visualisation experiments

Some visualisation experiments were carried out to find out whether the flow patterns that emerged from the numerical calculations could also be observed in our set-up. We used the laser-sheet visualisation technique mentioned earlier (Fig. 4.4). To visualise the flow inside the cavity, we first filled it uniformly with smoke using nitrogen as a carrier gas. This means that at the beginning of gas injection through the chamber walls the entire chamber was filled with nitrogen and smoke particles. During gas injection the smoke was displaced from below by the injected argon. Nitrogen is injected through the (cold) side walls, and argon is injected through the hot base plate, to create opposed flow. Figure 4.11 shows a cross-section of the convection chamber at $D/2$. The smoke can be seen to lie flat on a transparent layer of the (heavy) argon, injected from below.

Figure 4.12 shows the argon iso-concentration lines for a simulation in which the gas injection rate was 0.08 mole/m$^2$/s. At the bottom of the domain, a thick layer with a high argon concentration is formed in the stationary situation. For the simulations, this layer is formed at higher injection rates than during the experiments. The visualisation experiments showed that already at low gas injection rates the flow inside the chamber became stratified, see Fig. 4.11. The same stratification also emerged from numerical simulations [7] at gas injection rates which were $\sim$3.5 times as high (see Fig. 4.12). It should be noted that for the numerical simulations, a large hysteresis effect was observed. Stratification was found for much lower injection rates when simulations were started at high injection rates.
Figure 4.11: Smoke visualisation experiment showing a smoke plume halfway down the cold side wall, pointing inward to the centre of the chamber. Gas injection rate is 0.023 mole/m²/s. The illuminated plane is located at half the cavity depth (D/2).

Figure 4.12: Simulation result showing argon iso-concentration lines. Gas injection rate is 0.08 mole/m²/s.
4.5.2 LDA measurements

Figures 4.13 and 4.14 show measured vertical and horizontal velocity profiles for different argon and nitrogen injection rates. We used equal injection rates for argon and nitrogen, starting at 0.003 mole/m²/s, up to 0.017 mole/m²/s. An increase in the injection rate corresponds to an increase in the Sherwood number. The effect of an increase in gas injection rate on the velocity profiles is clear: the maximum vertical velocities can be seen to decrease slightly. To a lesser extent, this also counts for the horizontal velocity profile. The effect of an increase in gas injection is, however, larger in the experiments than in the simulations (see Figs 4.15 and 4.16). Apart from this effect the horizontal measured velocities agree reasonably well with the simulations. Figure 4.17 shows a measured and simulated horizontal velocity profile for an injection rate of 0.01 mole/m²/s. The vertical velocity profile shown in Fig. 4.18 shows a considerable discrepancy between measurements and simulations: the measured velocities are structurally higher than the simulated velocities. A possible explanation for this could be a 3D effect induced by the permeable rear wall through which the injected gases leave the convection chamber.

![Graph](image)

Figure 4.13: Vertical velocity profiles, measured for five different gas injection rates. The legend indicates the injection rate in mole/m²/s. Profile at $y = 0.54H$. Table 4.2 lists the average wall temperatures.
CHAPTER 4. DOUBLE-DIFFUSIVE NATURAL CONVECTION

Figure 4.14: Horizontal velocity profiles, measured for five different gas injection rates. The legend indicates the injection rate in mole/m²/s. Profile at $y = 0.54 \mathcal{H}$. Table 4.2 lists the average wall temperatures.

Figure 4.15: Vertical velocity profiles, simulated for eight different injection rates. The legend indicates the injection rate in mole/m²/s. Profile at $y = 0.54 \mathcal{H}$. Table 4.2 lists the average wall temperatures.
4.5. DOUBLE DIFFUSIVE NATURAL CONVECTION

Figure 4.16: Horizontal velocity profiles, simulated for eight different injection rates. The legend indicates the injection rate in mole/m$^2$/s. Profile at $y = 0.54H$. Table 4.2 lists the average wall temperatures.

Figure 4.17: Horizontal velocity profile, measured (symbols) and simulated (drawn line). The legend indicates the injection rate in mole/m$^2$/s. Profile at $y = 0.54H$. Table 4.2 lists the average wall temperatures.
4.6 Conclusions

- Visualisation experiments with a temperature driven natural convection flow show that the flow behaviour in the trapezoidal chamber is essentially two-dimensional, and can therefore be compared with two-dimensional numerical calculations.

- Temperature driven measurements compare fairly well with calculations, albeit that the measured vertical velocity profiles show some asymmetry.

- Double-diffusive LDA measurements show that an increase in gas injection rate slows down the flow in the trapezoidal chamber. This slowing-down effect can also be seen in the numerical simulations, but only at much higher gas injection rates.
4.7 Nomenclature

Latin
\( \mathcal{D} \) = depth of the trapezoidal convection chamber, L, m
\( \mathcal{D} \) = molecular diffusion coefficient, L\(^2\) / t, m\(^2\) / s
\( Gr \) = Grashof number
\( g \) = gravitation vector, L / t\(^2\), m / s\(^2\)
\( H \) = height of the trapezoidal convection chamber, L, m
\( k \) = turbulent kinetic energy, L\(^2\) / t\(^2\), m\(^2\) / s\(^2\)
\( Pr \) = Prandtl number
\( Ra \) = Rayleigh number
\( Sc \) = Schmidt number
\( Sh \) = Sherwood number
\( T \) = temperature, T, K
\( u \) = horizontal velocity component, \( (u = \overline{u} + u') \), L / t, m / s
\( v \) = vertical velocity component, \( (v = \overline{v} + v') \), L / t, m / s
\( w \) = transverse velocity component, \( (w = \overline{w} + w') \), L / t, m / s
\( W \) = width of the trapezoidal convection chamber, L, m
\( x \) = horizontal coordinate (positive in direction of \( u \))
\( y \) = vertical coordinate (positive in direction of \( v \))
\( z \) = transverse coordinate (positive in direction of \( w \))

Greek
\( \beta \) = thermal expansion coefficient, 1 / T, 1 / K
\( \delta_{ij} \) = Kronecker delta
\( \mu \) = dynamic viscosity, m / Lt, Pa s
\( \rho \) = density, m / L\(^3\), kg / m\(^3\)
\( \omega \) = mass fraction

Subscripts
\( c \) = cold
\( h \) = hot
\( i, j \) = coordinate index
\( n \) = normal
\( t \) = turbulent
\( T \) = temperature
CHAPTER 4. DOUBLE-DIFFUSIVE NATURAL CONVECTION
Bibliography


Chapter 5

High-pressure gasification experiments

In this chapter high-pressure and -temperature coal gasification experiments are described. The experiments were designed to demonstrate an indirect reaction sequence in which injected oxygen first reacts with combustible gases to form a hot gas which is in turn transported to the coal face and reacts there with coal to form combustible gas. These combustible gases partly react with the injected oxygen, and are partly produced via the production well. The experiments did not yield conclusive evidence of the reaction sequence proposed above. Numerical calculations indicate that higher coal-face temperatures are necessary to enhance the reaction rates at the coal face and sustain the proposed indirect reaction sequence.

5.1 Introduction

In an underground coal-gasification cavity or channel, heat and mass transfer, chemical reactions, and the flow of gases determine the behaviour of the gasification process. Since the process in the field takes place at great depth, it is extremely difficult to monitor and control the flow of gasifying agents and the temperature distribution in situ [1, 2]. This has an adverse effect on the interpretation of field-test results. Experiments under in-situ conditions in which monitoring of all the parameters of interest is possible would certainly aid in the interpretation and extrapolation of past and present field trials.

During a typical gasification process, the objective is to obtain a beneficial reaction sequence in the UCG-reactor (see Fig. 5.1). Upon entering the reactor, the injected air will react with combustible gases present inside the cavity under oxidizing conditions to form carbon dioxide. It is asserted that the relatively hot carbon dioxide rises to the upper part of the cavity and deflects to the side walls of the coal to react endothermically and form carbon monoxide \((\text{CO}_2 + \text{C} (s) \rightarrow 2\text{CO})\) [3]. The relatively cold carbon monoxide descends and serves partly as a reaction agent for the injected air and is partly produced via the production well. A more elaborate description of the flow inside the cavity can be found in
Chapters 4 and 3.

Both in the field and in the laboratory, the combination of high pressures and temperatures is conducive to high chemical reaction rates and mass-transfer rates. The European Working Group defined a set of conditions which should be fulfilled in a 'model underground coal gasifier' [4]. They defined an optimal process pressure of 65 bar.

In order to obtain a better insight in the factors influencing the gasification process an experimental laboratory set-up has been constructed in which a careful assessment can be made of which combination of conditions leads to the reaction sequence proposed above.

![Diagram of a typical underground coal-gasification reactor](image)

Figure 5.1: At the left a cross-section of a typical underground coal-gasification reactor, showing regions where oxidizing and reducing conditions prevail, respectively. The right picture shows a schematic representation of the experimental gasification reactor.

The chapter starts with a description of the experimental set-up and the measurement techniques that were used. After this, experimental results are presented and discussed. Simple heat loss and stirred-tank calculations are used to aid in the interpretation of the experimental results. The measured gas compositions and temperatures, enable a comparison of the reactive natural convection flows that can be inferred from the experimental results, and results obtained from numerical simulation models in past and present studies [5, 6]. This comparison should
lead to a better understanding of the behaviour of reactive natural convection flows inside a high-pressure and -temperature coal-gasification reactor. Optimal process parameters can thus be defined for underground coal gasification under typical North-Western European conditions.

5.2 Experimental set-up

The heart of the set-up consists of a high-pressure vessel in which a reactor is mounted. In this reactor, under carefully controlled conditions, both temperatures and gas compositions can be measured on-line during high-pressure coal-gasification experiments. The height of the reactor \( H = 0.75 \) m and process parameters such as temperature and pressure favour the occurrence of reactive turbulent natural convection flows inside the gasification cavity. Because the Rayleigh number defined in Chapter 3, a measure for natural convection flow, is proportional to \( H \) to the power three, height is an important parameter.

The set-up consists of six main parts: the high-pressure vessel, the reactor, the pressure-control system, the safety system, the data-acquisition system, and the gas chromatograph. These parts are described separately below.

5.2.1 High-pressure vessel

The pressure-vessel is a 1900 mm long cylinder of ASTM-A106-Grade-B steel, with an outside diameter of 323.8 mm and a wall-thickness of 21.4 mm. The vessel with a volume of 118 dm\(^3\) is fixed midways to a steel frame which allows the vessel to rotate and the reactor to be mounted into the vessel.

On each end, the cylinder has a welded neck flange with a 12 inch ring-joint facing, according to ANSI B 16.5. The vessel is closed by mounting two lids with twenty bolts M36 each. Each lid has five bushings for the regulation and registration of the processes inside, of which two bushings are used for the pressure control of the sand-filled annular space between the pressure vessel and the reactor.

5.2.2 Gasification reactor

Figure 5.2 shows a schematic representation of the gasification reactor. During an experiment, gas compositions and temperatures are determined at several points inside a vertically mounted reactor. The reactor itself does not have to be able to withstand high pressures, as the pressure in the annular space between the high-pressure vessel and the reactor always exceeds the process pressure by a preset value of 4 bar. The reactor consist of a stainless steel tube 750 mm long and 215 mm in diameter. In the reactor two layers are placed: an insulating outer layer of cement and an inner coal layer. The coal layer consists of a mixture of
active carbon (75 weight%), cement (25 weight%) and methyl-cellulose (∼0.08 weight%).

The process conditions mentioned which favour the gasification process require the reactor to be heated to sufficiently high temperatures (above 1000 degrees Kelvin). To achieve this goal, we chose to fill the inside of the reactor with carbon grains, which are gasified in the preparatory heating phase before the start of the actual experiment. This has the additional advantage that the reactor is filled with a combustible gas mixture when all the carbon grains are gasified and the cavity has grown to its full size. Schematized cross-sections of the reactor are shown in Figs 5.3 and 5.2.

Sample unit

The sample unit, which is coated with a coal layer, is placed inside the reactor (see Figs 5.2 and 5.3). The sample unit is equipped with eight sample locations of which six are placed in three pairs, each at a different height: B & C at 31 cm, D & E at 50 cm, and F & G at 63 cm. The lowermost sample line, A, is placed at 3 cm from the bottom of the reactor. A sample line pair consists of one sample line ending at the coal face and one sample line ending in the centre of the reactor. Sample line A ends in the centre of the reactor. From the stream of produced gas from the top of the reactor, a sample can be obtained as well (line H). Four thermocouples are placed at the same height as the sample line pairs. Two other thermocouples are placed at sample line A and halfway between line A and sample line pair B-C.

Accuracy of the thermocouple measurements

The Chromel alumel thermocouples that were used throughout the experiments have an absolute accuracy of 4 degrees Kelvin, and a relative accuracy of 0.05 degrees Kelvin.

5.2.3 Pressure control system

All experiments are performed at a certain predetermined process pressure. This process pressure is the reference pressure for the pressure-control system, which is set with a pressure regulator. The reference pressure acts on the dome of a heavy-duty backpressure relief valve ("Heijnen"-valve). Once the outlet pressure of the reactor reaches the reference pressure, the "Heijnen"-valve starts releasing gas into the production system. In order to be able to conduct high-pressure experiments with different types of reactors which do not withstand high pressures, the annular pressure has to be maintained at a level which is approximately 4 bars higher than the process pressure. The required pressure difference is monitored by a pressure-difference transmitter. This device measures the actual pressure
5.2. EXPERIMENTAL SET-UP

Figure 5.2: Cross-section (chamber: 0.75×0.14 m²) in side view of the gasification reactor, with sample line and thermocouple locations (TC) indicated.

difference and compares it with the preset value. Together, the “Heijnen”-valve and two pressure regulation valves, maintain the pressure difference between the annulus and the reactor.

5.2.4 The safety system

In case of an emergency shutdown, all pressures are released. All “Heijnen”-valves open and all the gases in the reactor are released into the drain. The safety system is capable of handling 32 channels. All thermocouples and pressure transducers are connected to this safety system. For each channel a minimum and a maximum analog value can be set. If a value is not in the preset range, the system sounds an alarm that has to be switched off within a delay time of five minutes. If not, the power will be cut off.

Whenever a design pressure or a maximum safety level is exceeded, the safety system immediately comes into effect. Without delay, emergency shutdown takes place. In case of an emergency, a red button can be pushed, to cut off the power supply.
5.2.5 The data-acquisition system

The data acquisition system of the experimental set-up can be divided into several features: temperature measurement, pressure measurement, flow measurement and gas composition analysis. When data are measured, signals are transferred into voltages, which are then transferred and amplified into signals in an appropriate range (0-4 Volt).

Thermocouples (type K, Chromel alumel) measure the temperatures inside the reactor, the produced gas temperature and the outside wall temperature of the pressure vessel. The 0-35 bar pressure devices record the injection and production pressure and the 0-1 bar pressure devices are used to convert the pneumatic signals of the flow controller. The signals are amplified to a 0-10 Volt range before entering the safety system. Amplification factors for the thermocouples, the 0-35 bar and the 0-1 bar pressure devices are 200, 50, and 100, respectively.

5.2.6 The gas chromatograph

The gas samples are analysed by a gas chromatograph which detects the difference in thermal conductivity between the carrier gas and the individual gas-sample components. A gas sample is injected into the column in which it is separated into the individual components [7, 8]. In this experimental set-up the CP2002 gas analyzer made by Chrompack, is used. This gas analyzer is equipped with two columns. The first is the HayeSep A column, which can detect air, methane and carbon dioxide. The second column is the PLOT Moleculesieve 5Å. This
Table 5.1: Average gas content after calibration.

<table>
<thead>
<tr>
<th>species</th>
<th>gas content [vol.%]</th>
<th>exp. gas content [vol.%]</th>
<th>dev. [%]</th>
<th>st. dev. [%]</th>
<th>99.73% conf.int. [vol.%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>10.2</td>
<td>10.3</td>
<td>1.0</td>
<td>0.34</td>
<td>±0.023</td>
</tr>
<tr>
<td>O₂</td>
<td>21.0</td>
<td>20.6</td>
<td>-0.64</td>
<td>0.27</td>
<td>±0.013</td>
</tr>
<tr>
<td>N₂</td>
<td>59.8</td>
<td>59.8</td>
<td>-0.018</td>
<td>0.30</td>
<td>±0.020</td>
</tr>
<tr>
<td>CH₄,A*</td>
<td>10.0</td>
<td>10.0</td>
<td>0.038</td>
<td>0.22</td>
<td>±0.015</td>
</tr>
<tr>
<td>CH₄,B*</td>
<td>10.0</td>
<td>10.1</td>
<td>0.80</td>
<td>0.35</td>
<td>±0.023</td>
</tr>
<tr>
<td>CO</td>
<td>10.0</td>
<td>9.87</td>
<td>-1.2</td>
<td>0.47</td>
<td>±0.031</td>
</tr>
<tr>
<td>CO₂</td>
<td>10.0</td>
<td>10.1</td>
<td>0.74</td>
<td>0.30</td>
<td>±0.020</td>
</tr>
</tbody>
</table>

1 oxygen is calibrated with air  * methane is determined at each of the two columns

column can separate hydrogen, oxygen, carbon monoxide, nitrogen and methane. The column conditions are controlled by a PC in which the gas-composition data are stored as well.

The lines from which the samples are taken are selected either by manual remote control or by a user program, operating an eight-way sampling valve.

Accuracy of the gas-composition measurements

Before an experiment is conducted, the gas chromatograph is calibrated with calibration gas, obtained from Scott Specialty Gases b.v.. The calibration gas used consists of 10.0 vol.\% carbon dioxide, 10.0 vol.\% carbon monoxide, 10.2 vol.\% hydrogen, and 10.0 vol.\% methane, balanced with nitrogen. The company guarantees a 5% analytical accuracy. With our gas chromatograph a repeatability test of 12 measurements was carried out to determine the experimental error in the determination of the gas composition. The experimental error is a combination of the systematic error and the standard deviation. Calibration is used to systematic errors in the measurements. The results are shown in Table 5.1. The strict 99.73% confidence intervals of the single measurement shown are for normally-distributed scattered measured values, see, e.g., Sydenham [9]. The calibration of the oxygen content was done with air\(^1\). These results prove that the deviation as well as the random errors fall well within the 5% analytical accuracy of the calibration gas. Assuming a worst-case scenario, the accuracy of determination of the gas content will be 5%.

\(^1\)21 vol.\% oxygen and 79 vol.\% nitrogen
5.3 Experimental procedure

In the course of this study eight successful experiments were carried with the high-pressure set-up. Various reactors and sample units were used, and different experimental boundary conditions were applied, in order to reach the optimal temperature level inside the reactor. Here we will highlight only one of the experiments, since the temperature and gas composition behaviour showed similar behaviour during all experiments.

The experiment we discuss here was carried out at a process pressure of 55 bar, with an average air injection rate of 0.04 Nm$^3$ / min. Initially the reactor with the coal layers fixed in place is filled with carbon grains and mounted inside the pressure vessel. After testing for possible leaks the pressure vessel and the reactor are filled with nitrogen to prevent untimely ignition of the coal. The pressure vessel is now preheated from the outside with heating elements for a period of several days to a temperature of $\sim$450 degrees Kelvin.

At the starting point of the preparatory heating phase the pressure vessel and the reactor are brought to the desired process pressure with nitrogen. When the process pressure is reached and there are no leaks, the heating element inside the reactor (shown in Fig. 5.2) is switched on. Air is carefully injected at a low rate and ignition of the carbon grains takes place near the injection point. For the next twelve hours air is injected and gas compositions and temperatures are monitored. From the thermocouple readings the size of the cavity can be inferred from the temperature difference between the permeable carbon grain pack and the cavity.

In Fig. 5.4 the development of the cavity inside the reactor is shown during the preparatory permeable-bed-gasification (heating) phase prior to a typical experiment. Air is injected from below, and the carbon grains are gasified from below as well. Since the carbon grains are loosely packed, a cavity will start to form at the top of the reactor, slowly growing in time as the heating phase progresses. During this heating phase, hydrogen will be formed in the reactor from the water that is present in the fixed coal layer and the cement protective layer. At the end of the heating phase, when all carbon grains are gasified, the cavity is filled with a mixture of nitrogen, carbon monoxide, carbon dioxide, and hydrogen. The end of the heating phase is reached shortly after the lowermost thermocouple reading drops. Now, the combustible gases present in the reactor will react directly with the oxygen in the injected air, to form carbon dioxide.

5.4 Experimental results

Figure 5.5 shows the thermocouple readings during the experiment. Since air injection takes place at the bottom of the reactor, the temperature readings are usually highest here (thermocouple 1). The initial stages of the heating
Figure 5.4: Development of the cavity inside the reactor in time during the preconditioning (heating) phase of an experiment.

period, however, show erratic behaviour of the thermocouple readings, indicating that during the first two hours the combustion zone may have been located as high as thermocouple number three (31 cm above the injection point). This can probably be attributed to small channels forming in the coal grain bed along which combustion takes place, leading to higher temperatures above the injection point. After approximately two hours, the readings of the thermocouple at the bottom are higher than the other thermocouple readings, and remain so for the duration of the heating phase, indicating that the combustion zone is now located at the bottom of the reactor.

Gas composition readings for each of the eight sample locations are depicted in Fig. 5.6. All composition paths show similar behaviour in time. In the early stages of the experiment, line A shows slightly different behaviour which is probably a result of the fact that the combustion zone initially forms along small channels in the carbon grain pack.

When all carbon grains are gasified, after approximately twelve hours, the now open reactor is filled with a hot gas consisting of roughly 20 vol.% CO, 10 vol.% CO₂, and 2 vol.% H₂. This composition is almost constant throughout the reactor, as can be seen in Fig. 5.6, in which the gas composition readings from all eight sample locations are shown. The cavity's temperature is nearly constant as well: approximately 800 degrees Kelvin.

Using a simple heat-loss model, we can calculate the temperature inside the carbon-grain-filled reactor, the temperature of the surroundings, and the temper-
Figure 5.5: Measured temperature profiles in the reactor during experiment VII. Thermocouple locations are shown in Fig. 5.2.
Figure 5.6: Measured concentration profiles [vol.%] versus time, Experiment VII. × = CO, Δ = CO₂, ◦ = H₂, and + = O₂.
ature inside the growing cavity (Fig. 5.4). A detailed explanation of the model and the equations is presented in Appendix 5A. As a result of the symmetry of the domain we only have to consider half the geometry.

Figure 5.7 shows calculated temperature profiles inside the (half)reactor, its surroundings, and the growing cavity. The highest temperatures are reached where the air is injected and subsequently carbon-grain combustion takes place; at the bottom of the reactor. Once all coal grains are gasified, the heat source at the bottom of the reactor is turned off, which would result in a dramatic temperature drop for the entire reactor. Such a temperature drop, however, does not take place in the experiment, because oxygen starts reacting directly at the coal walls after all combustible gases are burnt, producing heat.

The temperature at the bottom of the reactor was matched to the experimental value (see Fig. 5.5) by adjusting the (effective) heat losses to the surroundings. The calculated cavity temperatures show qualitative agreement with the experimental values, reaching values of approximately 800 degrees Kelvin after 11 hours of coal combustion. After the heating phase, the model is no longer valid.

Once all carbon grains are gasified, the gas composition changes dramatically (see Fig. 5.6). The gas is stripped of all its combustible components, CO and $\text{H}_2$, by the continued air injection. When all combustible gases are gone, oxygen breakthrough takes place in the reactor. Now, part of the oxygen must react at the coal walls to form carbon dioxide, since this gas continues to be measured and produced.

Assuming a direct reaction of oxygen with combustible carbon monoxide and hydrogen in the reactor, we can calculate the decline in carbon monoxide and hydrogen concentrations, and the rise in carbon dioxide concentration. For these calculations we used a \textit{continuous-stirred tank} approximation. Details are presented in Appendix 5B. Figure 5.8 shows the calculation results. One can see from the figure that the CO and $\text{H}_2$ decline and the CO$_2$ rise match for only a limited period of time. After oxygen breakthrough, the assumptions on which the calculations are based are no longer valid.

It should be noted that carbon dioxide continues to be produced at a more or less constant level after all carbon monoxide has been consumed (Fig. 5.6). This means that part of the injected oxygen reacts directly at the coal face, forming carbon dioxide.

### 5.5 Discussion

We can, using a simple heat-loss model, calculate the temperatures inside the reactor during the preparatory heating phase of the experiment, including a growing cavity inside the reactor. A detailed derivation of the model equations is given in Appendix 5A. Since the flow in the reactor is well-mixed, we can simulate the
Figure 5.7: Calculated temperature distribution and cavity growth in time. The narrow band at the left of each picture represents the reactor, with the cavity indicated by a hatched area.
decline in combustible gas concentrations and the rise in the CO$_2$ concentration at the end of the heating phase using a continuous-stirred tank approximation.

Unfortunately, our experiments did not show evidence of the sequence of reactions proposed in the introduction of this chapter. Both cavity and wall temperatures were too low at the end of the heating phase to sustain a high enough reaction rate for carbon dioxide at the coal walls. Either higher wall temperatures or a higher reaction rate could possibly overcome this problem.

Numerical calculations performed by Kuyper [5] and Van der Eyden [6] indicate that wall temperatures in the order of 1000 degrees Kelvin would suffice to keep the reaction mechanism going. Using our experimental wall temperatures, their calculations also lead to very poor gas qualities.

5.6 Conclusions

- Under our experimental conditions the results show no evidence of a mech-
anism in which carbon dioxide reacts at the coal face to produce carbon monoxide. This can be attributed to too low wall temperatures, resulting in too low a reaction rate at the coal face for carbon dioxide.

- The high pressure gasification experiments showed that both the presence of water and transient heat losses have a detrimental effect on the final temperatures.
Bibliography


Appendix 5A

Heat losses during coal combustion

At the start of an experiment, the reactor is filled with coal grains, forming a porous medium. After ignition by a heating element the coal grains are combusted from below as a result of air injection, see Fig. 5A.1. Purpose of this coal combustion phase is to heat the reactor to sufficiently high temperatures for reactive natural convection flow to occur, once all coal grains are combusted, and to improve the reaction rate of carbon dioxide at the coal walls.

Figure 5A.1: Vertical cross-section of the reactor showing the cavity, coal grain filling, and the combustion zone at the bottom of the reactor.

Following Bruining [10], we can derive an equation for heat flow by convection and conduction in a porous medium, including heat exchange between the
medium and its surroundings.

\[
\begin{align*}
\text{heat conduction flow direction} & \quad \text{temperature change solid} \\
\frac{k}{\partial x^2} T_s & - \rho_s c_s (1 - \phi) \frac{\partial T_s}{\partial t} & + \\
\text{heat supplied to solid} & \quad \text{heat conduction to surrounding} \\
\frac{v_g \rho_g \Delta H}{\rho_{\text{air}} 4.77} \delta(x) & + \left. \frac{\lambda}{b} \frac{\partial T}{\partial y} \right|_{y=b} = 0
\end{align*}
\]

(5A.1)

and for the gas:

\[
\begin{align*}
\text{temperature change gas} & \quad \text{heat from gas to volume} \\
- \phi \rho_g c_g \frac{\partial T_g}{\partial t} & - v_g \rho_g c_g \frac{\partial T_g}{\partial x} = 0
\end{align*}
\]

(5A.2)

In which we have assumed that the temperatures of gas and solids are equal. At the cavity boundary, the effective heat transfer is determined by the flow characteristics inside the cavity. Now, adding equations 5A.1 and 5A.2, and neglecting heat conduction in the flow direction leads to:

\[
\rho_m c_m \frac{\partial T}{\partial t} + v_g \rho_g c_g \frac{\partial T}{\partial x} - \left. \frac{\lambda}{b} \frac{\partial T}{\partial y} \right|_{y=b} = \frac{v_g \rho_g \Delta H}{\rho_{\text{air}} 4.77} \delta(x), \quad y \leq b(5A.3)
\]

The heat conduction to the surroundings of the reactor is described by:

\[
\lambda \frac{\partial^2 T}{\partial y^2} = \rho_b c_b \frac{\partial T}{\partial t}, \quad y \geq b(5A.4)
\]

in which \(\lambda\) and \(\rho_b c_b\) are the (effective) thermal conductivity and heat capacity of the surroundings, respectively. Equations 5A.3 and 5A.4 can, after some manipulation, be written in dimensionless form:

\[
\frac{\partial T_D}{\partial t_D} + \frac{\partial T_D}{\partial x_D} - \frac{\partial T_D}{\partial y_D} = \delta(x_D), \quad y_D \leq 1(5A.5)
\]

\[
m \frac{\partial^2 T_D}{\partial y_D^2} = \frac{\partial T_D}{\partial t_D}, \quad y_D \geq 1(5A.6)
\]

The dimensionless variables are:

\[
\begin{align*}
x_D &= \frac{\lambda x}{v_g \rho_g c_g b^2} \\
y_D &= \frac{y}{b}, \\
T_D &= \frac{\left( T - T_0 \right)}{T_{\text{ref}}} \\
t_D &= \frac{\lambda t}{\rho_m c_m b^2} \\
m &= \frac{\rho_m c_m}{\rho_b c_b}
\end{align*}
\]
Initial conditions for the problem are:

\[ T_D(x_D = 0, t_D) = 0 \text{ and } T_D(x_D, t_D = 0) = 0 \]

We used a finite-volume method to solve this set of equations numerically, and to obtain the temperature field inside the domain. Table 5A.1 lists the main input parameters that were used in the calculations.
Appendix 5B

Stirred-tank calculations

To aid in the interpretation of the experiment, we performed some simple calculations to model the gas concentrations that were measured during the experiment. Since there is hardly any difference visible between the gas compositions measured (in the cavity, not in the porous coal grain pack) at the various sample locations, we can suffice with a so-called continuous-stirred-tank-reactor approximation. Indeed the natural convection flows inside the reactor will lead to a well-mixed, virtually uniform distribution of gas composition.

Continuous-stirred tanks are very common in the chemical process industry. Here we present a simple model on which the gas-composition calculations are based, following Aris [11] and Scott-Fogler [12]. The basic principle is simple: a tank filled with a well-mixed fluid at t=0 is injected with another fluid, the two fluids mix, chemical reactions take place and a product fluid is produced. A schematic representation of such a process is shown in Fig. 5B.1. The reactor volume is constant in our case. Upon entering the reactor, oxygen will react with the carbon monoxide present to form carbon dioxide: 2CO + O₂ → 2CO₂. We can write down expressions for the concentration change of the gas species of interest:

\[
\begin{align*}
\frac{d[CO]}{dt} &= -2\alpha Q_{\text{air}} \frac{P}{fV \frac{RT}{f}} - \frac{Q_{\text{air}} [CO]}{fV} \\
\frac{d[CO_2]}{dt} &= \alpha Q_{\text{air}} \frac{P}{fV \frac{RT}{f}} - \frac{Q_{\text{air}} [CO_2]}{fV} \\
\frac{d[H_2]}{dt} &= -2(1 - \alpha) Q_{\text{air}} \frac{P}{fV \frac{RT}{f}} - \frac{Q_{\text{air}} [H_2]}{fV}
\end{align*}
\]  

(5B.1)

in which the gas species between square brackets denotes concentration, V is the reactor volume, f is the fraction of oxygen in air, P the pressure, R the gas constant, Q_{\text{air}} the air injection rate, \alpha (a value of 0.9 gave the best match with experimental results) is the fraction of the oxygen which reacts with carbon monoxide, and T the (average) temperature.
Figure 5B.1: Schematic representation of a continuous-stirred tank reactor. Note that $Q_{\text{out}} = Q_{\text{in}}$
Chapter 6

Simulations of past field trials

In this chapter two field trials are simulated and evaluated using the model developed and presented in Chapter 2. Both a field trial in a thick, and a field trial in a thin coal layer are evaluated. Model results show that when mass transfer rates are relatively high and the exposed cavity surface is large, a cylindrical cavity develops in the coal seam. When the exposed cavity surface is considerably smaller and surface gasification plays a minor role, the permeability distribution of the coal largely determines cavity development, leading to a teardrop-shaped ash/rock rubble pile in the centre of the gasification channel.

6.1 Introduction

We use the three-dimensional model developed and presented in Chapter 2 to simulate two past field trials. This serves two purposes: firstly, calibration of the model with known field-test results, and secondly, extrapolation of the field-test results to deep-lying thin coal seams such as exist in North-Western Europe.

Our base case simulations presented in Chapter 2 showed that, for a representative combination of input parameters, natural-convection-driven cavity-surface gasification is of the same order of magnitude as the direct gasification. Local mass-transfer rates, and the exposed coal surface were combined into a simple model. Chapters 3 and 4 show that a uniformly distributed value of the mass transfer coefficient is a good approximations for the natural convection typical for underground coal gasification. In typical field cases, however, the relative importance of these processes can vary strongly, depending on both the process parameters and the coal properties.

We selected two field trials for simulation, i.e., the Rocky Mountain I and the Pricetown test. The Rocky Mountain trial was chosen since it is both well-documented and representative for the American situation with a thick (7.6 m), flat-lying shallow coal seam. The Pricetown field test was conducted in a relatively thin (1.8 m) coal layer, which is more in line with the North-Western European situation. Since most UCG field trials are well-documented, it is relatively easy to distill the necessary input parameters from the literature.
6.2 Rocky Mountain field test

In mid-November 1988, a field test started in the Rocky Mountains, Wyoming, U.S.A., to investigate the viability of underground coal gasification in a thick (7.6 m), flat-lying, subbituminous coal seam. The test ran for about 100 days. The test programme was jointly sponsored by the U.S. Department of Energy, Morgantown Energy Technology Center and an industry consortium led by the Gas Research Institute. The programme was managed by the Stearns-Roger Division of United Engineers and Constructors, Inc. Related research was carried out by Lawrence Livermore National Laboratories, Western Research Institute, North Dakota Mining and Mineral Resources Research Institute, Energy International, Inc., and the Project Construction Corporation [1].

The trial consisted of the simultaneous operation of two gasifiers: the Controlled Retraction of Injection Point module (CRIP), and the Extended Link Well (ELW) module. The CRIP operation proved to be successful during a 100 day period, in which the injection point was retracted three times. The Extended Link Well module failed during operation and will not be discussed here.

For the entire CRIP module more than 11,000 tonnes of coal were gasified, with an average heating value of produced gas of 10,700 [kJ / m³] [2]. CRIP test operations consisted of air-acceptance testing, dewatering of the formation, linking, stabilization, oxygen gasification, CRIP manoeuvres, and finally shutdown. Problems occurred with respect to steam production, flow measurement, freezing, and oxygen-flow control, but in general the design of the facilities met the operating parameters specified [1-3].

The field-test results showed that the CRIP process was competitive with surface gasification, when gas composition, plant costs, and operating costs are considered [4,5].

As a tool for the interpretation of this field trial, Britten and Thorsness developed a model for calculating cavity development during UCG [6]. Their 'CAVSIM' (cavity simulator) model relies on a few basic assumptions: (1) the cavity is axisymmetric about the injection point, (2) all resistance to injected gas flow is through ash and overburden rubble, (3) thermal radiation dominates in the well-mixed void, and (4) coal and overburden spall as a result of thermal effects, on a small scale. Using this model, the cavity that was formed during the first CRIP step was simulated and compared with the actual field data. We used their CAVSIM model for comparing the resulting cavity shape with our own modelling results.

6.2.1 Simulation results: Rocky Mountain I

In Table 6.1 we show the input parameters that we used to simulate the first CRIP step. We used the same permeability values and ratios as Britten and Thorsness in their CAVSIM simulation study [7]. The estimated parameters
such as the reaction rate, r, and the number of moles carbon affected by a mole of injected reactant, P, were based on the simple models described in Chapter 2. The process pressure and temperature largely determine these quantities. The injection/production well configuration is shown in Fig. 6.1.

![Diagram of injection/production well configuration](image)

Figure 6.1: Rocky Mountains field trial: Injection/production well configuration. $h \times L \times W = 7.6 \times 20 \times 20$ m$^3$, on a $16 \times 16 \times 16$ grid.

Figure 6.2 shows the fraction of the coal initially in place gasified as a result of (natural-convection-driven) surface gasification and the fraction gasified as a result of direct gasification (permeable-bed gasification, including coal spalling) plotted against the total amount of coal gasified. It is clear that the relative importance of surface gasification increases with the increase of the cavity’s exposed coal surface. As soon as 10% of the coal has been gasified, surface gasification becomes more important than permeable-bed gasification combined with coal spalling.

Figures 6.3 and 6.4 show the cavity shape and ash distribution for our calculations after 26.5 and 33 days, respectively. The coal and rock spall rate were taken 10/256, i.e., 10 pairs of random numbers are drawn for a total of 256 columns for each time step. This way we matched both the volume of coal affected and the moment the cavity reached the overburden (roof rock) during the field test, after approximately 21 days in the first CRIP-step. The cavity shape is very much influenced by the ash/coal permeability ratio. Indeed virtually any shape can be obtained by controlling the spall rates and the ash/spalled rock permeability [7].

The simulation results show that a relatively smooth cavity develops inside the coal. The natural convection driven surface gasification which is distributed uniformly over the coal’s surface is the main cause for this. The ash/rock rubble pile forming at the injection point covers the injection point at the bottom of the cavity. The volume of affected coal matches the field-test results very closely, since the same gradually increasing injection rate configuration was used [3].
Initial and final velocity distributions are shown in Fig. 6.5. Once breakthrough in the production well occurred, surface gasification and spalling are the only means by which coal can be affected. The reason for this is that most of the injection gas flows through an already gasified zone, which effectively prohibits direct gasification. At this point in time, injection rates would have to be lowered to prevent oxygen breakthrough in the production well.

The shape of the cavity that formed during our model calculations is similar to the cavity resulting from our calculations using Britten and Thorsness' model [6]. Figure 6.6 shows a picture of the cavity cross-section after 26.5 days of gasification simulation with the CAVSIM simulator and our simulator. Contrary to the CAVSIM model, our model does not impose a radial symmetric upward and outward growth of the cavity, originating at the injection point. We used the spall rate of coal and rock to match the amount of coal affected and the moment the roof rock is reached. The picture of the CAVSIM simulation does not show the outflow channel, which in their model accounts for about 10% of gasification.
Figure 6.3: Rocky Mountain I CRIP: 3D view showing the gasified region (left picture) and the ash/spalled rock region (right picture) after 26.5 days of gasification. The top half (roof rock) region is not shown in the figure.

Figure 6.4: Rocky Mountain I CRIP: 3D view showing the gasified region (left picture) and the ash/spalled rock region (right picture) after 33 days of gasification. The top-half (roof rock) region is not shown in the figure.
Figure 6.5: Rocky Mountain I CRIP: 3D view showing the initial velocity distribution (left picture) and the end time velocity distribution (right picture), showing high velocities near the production well in which breakthrough has occurred.

Figure 6.6: Comparison of simulators. Cavity formed after 26.5 days of gasification as a result of a CAVSIM simulation of the Rocky Mountain I first CRIP step (drawn lines). The CAVSIM simulation is projected on a cross-section of the cavity and the ash/rock rubble pile obtained with our simulator (darker shaded area = cavity, lighter shaded area = ash/rock rubble).
Table 6.1: Input parameters for the first CRIP step of the Rocky Mountains field trial. Reasonable values were adopted for unknown parameters. For an explanation of the symbols please refer to the Nomenclature at the end of Chapter 2.

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<td>(estimated)</td>
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$^1$standard conditions: $1 \cdot 10^{5}$ Pa, 293 K
Figure 6.7: Pricetown field trial: Injection/production well configuration. \( h \times L \times W = 1.8 \times 25 \times 12.5 \text{ m}^3 \), on a \( 16 \times 32 \times 16 \) grid.

6.3 Pricetown I field test

In October 1979, an underground coal-gasification field trial was conducted in a relatively thin (1.8 m) flat-lying, bituminous coal, located at a depth of 274 m. The field trial was performed by the Morgantown Energy Technology Center of the U.S. Department of Energy, in cooperation with the Industrial Environmental Research Laboratory of the Continental Oil Company. The Pricetown I field test consisted of seven phases [8]: (1) pre-ignition tests, (2) coal-seam ignition, (3) reverse combustion linkage, (4) link enhancement, (5) gasification, (6) post gasification/test termination, and (7) post-burn evaluation. During the reverse combustion-linkage phase, considerable difficulties were experienced with buildup of tars and oils in situ. These problems were resolved in the so-called link enhancement phase by interchanging the injection and production wells to burn away the heavy substances. In this way, the permeability of the linkage path was increased to permit the high gas-flow rates that are required for gasification.

The forward gasification phase itself was a success until on day 12 a casing ruptured in the production well. The test had to be terminated at this stage because the leak caused a near-surface aquifer to be pressurized. After pressure was relieved and the test was terminated, surface-, shallow-, and deep-water quality were monitored for a period of two years.

6.3.1 Simulation results: Pricetown I

For the simulations we confine ourselves to the gasification phase (5). Table 6.2 lists the relevant input parameters that could be obtained from the gasification results [8], and the operating conditions during the field trial. In Fig. 6.7 the injection/production well configuration is depicted. Prior to the forward gasific-
Table 6.2: Input parameters for the gasification phase of the Pricetown I field trial. Reasonable values were adopted for unknown parameters. For an explanation of the symbols please refer to the Nomenclature at the end of Chapter 2.

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$^1$standard conditions: $1 \cdot 10^5$ Pa, 293 K
Figure 6.8: Pricetown field trial: Fraction of coal initially in place gasified as a result of surface gasification and coal gasified as a result of direct gasification (permeable-bed gasification including coal spalling) versus the total amount of coal gasified.

Gasification phase, a reverse-combustion link was created to char the coal, enhancing the permeability. The linkage permeability was determined from pre-gasification pressure and rate data. We chose a simple link geometry at $W/2$, 0.78 m (one gridblock) wide over the entire height of the coal layer.

We calculated the cavity shape resulting from the gasification phase, step (5). In Fig. 6.8, surface gasification is plotted versus permeable-bed gasification including coal spalling are plotted versus total gasification. From the figure we can see that the ratio of surface gasification and permeable-bed gasification/coal spalling remains more or less constant. Due to a small exposed cavity surface, natural-convection-driven surface gasification never becomes more important than permeable-bed gasification including coal spalling.

Figure 6.9 shows the cavity shape interpreted from post-field-trial coring at the end of the forward gasification phase [9]. Figure 6.10 shows the final cavity shape and ash distribution, after 12 days of gasification. To match the amount of coal gasified, we used a coal and rock spall rate of 10/512 (10 pairs of random numbers $\mathcal{R}$ are drawn for the total of $16 \times 32 = 512$ columns). The top of the ash/rock rubble pile in the figure has grown above the pre-trial overburden level, an interpretation that was also made by Liberatore [8], from coring data. Comparing Figs 6.9 and 6.10 at the end time, we can observe a good agreement between field test data and modelling results. The modelled cavity shape is more
irregular than the smoothed cavity obtained from post-burn coring tests. The cavity shape is largely determined by the initial permeability field, since surface gasification plays only a minor role during gasification. Figure 6.11 shows both the initial and final velocity distribution in the simulation domain. The large velocities along the linkage-zone axis of enhanced permeability confirm the development of an elongated channel. The large velocities to all sides near the injection point, together with the coal-surface gasification account for the sideways growth of the cavity near the injection point.
Figure 6.10: Pricetown field trial: 3D view showing the gasified region (left picture) and the ash/spalled rock region (right picture) at the end time, after 12 days of gasification. The vertical scale has been exaggerated by a factor 6. The injection well is located at $(L/4, W/2, 0)$, production at $(L, W, 0-h/2)$.

Figure 6.11: Pricetown field trial: 3D view showing the initial velocity distribution (top picture) and the final velocity distribution (bottom picture). The vertical scale has been exaggerated by a factor 6.
6.4 Conclusions

- We have successfully simulated the performance of two US field trials using our UCG model. The rock and coal spall rates were used as matching parameters.

- Simulation of the Rocky Mountain I field trial shows the formation of a radial symmetric cavity. This can be attributed to the large exposed coal surface, combined with the relatively large surface mass-transfer coefficient $k_f$.

- Simulation of the Pricetown I field trial leads to a teardrop-shaped ash/rock rubble zone extending from the injection well towards the production well, surrounded by an open channel. This is the same gasifier geometry that was interpreted from field trial results.

- For successful gasification in thin coal layers as exist in North-Western Europe, the initial permeability field is very important, since this dominates the cavity shape before breakthrough and thus the amount of coal that can be gasified per injection/production well pair. After breakthrough, coal surface gasification and spalling will be the only modes of gasification by which the cavity develops.
Bibliography


Summary

Underground coal gasification (UCG) is a potentially attractive method for recovering the huge coal resources that cannot be mined using conventional methods. Deep-lying and thin coal seams can be accessed using standard horizontal drilling techniques, widely used in the oil industry. Coal is converted into a combustible gas \textit{in situ} by means of air injection. The gas produced is transported to the surface, where it can be used as fuel. Essential for the economic success of the gasification process is the attainable sweep efficiency per injection/production well pair.

In this study we focus on the development of an underground coal gasification cavity. We have developed an integrated 3D model for underground coal gasification. In addition, we have investigated the role of natural convection flows experimentally under various laboratory conditions.

In Chapter 2, the integrated 3D model for underground coal gasification is presented. The model includes aspects of permeable bed gasification, natural convection-driven cavity surface gasification and roof-failure mechanisms. Example calculations show that, for a representative combination of input parameters, a fairly high sweep efficiency is reached before breakthrough. With this model the influence of the various processes on the entire gasification process can be assessed.

In Chapter 3, we present Laser Doppler measurements in a rectangular differentially heated enclosed convection chamber. The experimental results in the form of velocity and turbulent kinetic energy profiles are compared with numerical calculations. A low-Reynolds turbulence model shows the best agreement with the measurements.

In Chapter 4, we present Laser Doppler measurements in a trapezoidal differentially heated chamber, in which differences in composition can also be introduced as driving force, in order to study \textit{double diffusive} natural convection flows. First, temperature-driven measurements are presented, as well as visualizations of the flow pattern inside the enclosure. LDA measurements compare well with numerical results. Finally, we present a limited number of measurements of the \textit{double diffusive} situation, in which temperature- and composition-driven natural convection flows are opposed.

In Chapter 5, high-pressure and -temperature coal-gasification experiments
are described. The experiments were designed to demonstrate an indirect reaction sequence in which injected oxygen first reacts with combustible gases to form a hot gas which is in turn transported to the coal face and reacts there with coal to form a combustible gas. Part of these combustible gases react with the injected oxygen, and the rest are produced via the production well. Our experiments did not show conclusive evidence of the reaction sequence proposed above. Numerical calculations indicate that higher coal-face temperatures are necessary to enhance the reaction rates at the coal face and sustain the proposed indirect reaction sequence.

In Chapter 6, two field trials are simulated and evaluated using the model developed and presented in Chapter 2. Both a field trial in a thick and a field trial in a thin coal layer are evaluated. Model results show that when a large surface area of coal is exposed and is available for surface gasification, and mass transfer rates are relatively high, a cylindrical cavity develops in the coal seam, an observation that was also made in the Rocky Mountain I field test. In the Pricetown field trial, where the exposed coal surface was small, and thus the overall mass transfer rate was considerably lowered, the coal permeability distribution largely determined cavity development, leading to a teardrop-shaped ash/rock rubble pile in the centre of the gasification channel. Simulation results show the development of a channel gasifier. This was also inferred from field test data and post-test coring results.

In general, it can be concluded that the model we have developed is a useful tool for interpreting field test results. The aspects of underground coal gasification which are taken into account lead to a model that describes overall cavity development from the initial stages to a mature gasifier. Using this model, we have successfully simulated two past field trials, one in a thick coal layer, and a thin coal layer, respectively. In thick coal layers the final cavity shape is mainly determined by the relatively large mass transfer at the coal face, resulting in a more or less cylindrical cavity shape. For thin coal layers, initial cavity development is largely determined by the linkage path that is created prior to the gasification phase.
Samenvatting (Summary in Dutch)

Ondergrondse kolenvergassing (OKV) is potentieel een aantrekkelijke methode om de enorme hoeveelheden steenkool te gebruiken die niet op de conventionele manier winbaar zijn. Diep gelegen en dunne kolenlagen kunnen worden ontsloten met behulp van uit de olie-industrie afkomstige standaard horizontale boortech- nieken. Bij deze methode wordt een kolenlaag in situ omgezet in een brandbaar produktgas door lucht te injecteren. Het produktgas wordt vervolgens naar de oppervlakte getransporteerd waar het als brandbaar gas gebruikt kan worden. Cruciaal voor het economisch succes van het vergassingsproces is de hoeveelheid kool die kan worden vergast per injectie/productieput paar.

Deze studie richt zich op de ontwikkeling van een ondergrondse vergassingsruimte. Een geïntegreerd drie-dimensionaal model voor OKV wordt ontwikkeld en gepresenteerd. Tevens wordt in drie experimentele opstellingen gekeken naar de rol die natuurlijke convectiestromen spelen bij het vergassingsproces.

In Hoofdstuk 2 wordt het geïntegreerde 3D model voor OKV gepresenteerd. Het model verenigt aspecten in zich van permeable bedvergassing, natuurlijke convectie gedreven oppervlaktevergassing, en thermomechanisch gedreven afsplin- tering van kool en dakgesteente. Uit voorbeeld modelberekeningen blijkt dat, voor een representatieve combinatie van invoergegevens, het vergassingsproces vóór doorbraak redelijk tot goed efficient te noemen is. Met dit model kan de invloed van de diverse deelprocessen op het totale vergassingsproces worden bepaald.

Hoofdstuk 3 behandelt Laser Doppler metingen in een rechthoekige differentieel verwarmde convectiekamer. De meetresultaten in de vorm van snelheidsprofielen en turbulente kinetische energie profielen worden vergeleken met numerieke berekeningen. Een laag-Reynoldsgetal turbulentiemodel geeft de beste overeen- komst met de metingen.

In Hoofdstuk 4 worden Laser Doppler metingen in een trapeziumvormige differentieel verwarmde convectiekamer gepresenteerd. In deze kamer kunnen ook samenstellingsverschillen worden geïntroduceerd als drijvende kracht voor natuur- lijke convectiestroming. Allereerst wordt een aantal temperatuurgedreven metingen gepresenteerd en vergeleken met numerieke resultaten. Ook wordt een aantal
visualisatie metingen gedaan, om het twee-dimensionale karakter van de stroming te verifiëren. De LDA-metingen komen goed overeen met de numerieke simulaties. Tenslotte wordt nog een beperkt aantal metingen gepresenteerd van de dubbele diffusie situatie waar temperatuur- en samenstellingsgedreven natuurlijke convectie elkaar in toenemende mate tegenwerken.

In Hoofdstuk 5 worden de hoge temperatuur en druk vergassingsexperimenten beschreven. Doel van deze experimenten was het aantonen van een indirect reactieproces waarbij zuurstof eerst met het in de holruimte aanwezige brandbare gas reageert tot een heet gas dat vervolgens naar de kolenwand wordt getransporteerd, en daar met kool reageert tot een brandbaar gas. Een deel van dit brandbare gas zal weer met de geïnjecteerde zuurstof reageren, een ander deel zal via de produktieput afgevoerd worden. De experimenten lieten geen overtuigend bewijs zien van het reactieproces zoals hierboven beschreven. Numerieke berekeningen geven echter aan dat een hogere temperatuur van de kolenwand nodig is om de reactiesnelheid aan deze kolenwand te verbeteren en het reactieproces aan de gang te houden.

In Hoofdstuk 6 wordt een tweetal veldtesten gesimuleerd en geëvalueerd met het in Hoofdstuk 2 ontwikkelde en gepresenteerde model. Zowel een veldtest in dikke kolenlaag als één in een dunne kolenlaag komen aan de orde. De modelresultaten laten zien dat wanneer de massaoverdracht relatief hoog is, en de voor oppervlaktevergassing beschikbare kolenwand groot is (dikke kolenlagen), zich een min of meer cilindrische holruimte vormt in de kolenlaag. Deze observatie werd ook gemaakt in de Rocky Mountain I veldtest. In de Pricetown veldtest, waar door de dunnere kolenlaag het aan oppervlaktevergassing blootgestelde kooloppervlak kleiner was en de massaoverdracht lager, werd de ontwikkeling van de holruimte grotendeels bepaald door de permeabiliteitsverdeling in de kolen. De simulaties van deze veldtest laten een druppelvormige as/puinkegel zien rondom het injectiepunt. Deze uiteindelijke vorm van de kanaalvergasser werd ook gehaald uit de interpretatie van veldtestresultaten en kernen die na de test zijn genomen.

Over het algemeen kan men concluderen dat het door ons ontwikkelde model van dienst kan zijn in de interpretatie en evaluatie van veldtestresultaten. De aspecten van ondergrondse kolenvergassing die worden meegenomen leiden tot een model dat de ontwikkeling van een vergasser beschrijft vanaf de initiële fase tot en met de volledig ontwikkelde fase. Met het 3D model hebben we twee in het verleden uitgevoerde veldtests succesvol kunnen simuleren: één in een dikke kolenlaag, en de ander in een dunne kolenlaag. In het geval van dikke kolenlagen wordt de uiteindelijke vergasservorm vooral bepaald door de massaoverdracht aan de kolenwand, en ontstaat een cilindersymmetrische vergassingsruimte. Bij dunne kolenlagen wordt de initiële vergasservorm voornamelijk bepaald door de verbinding die moet worden gemaakt in de kolenlaag vóór de eigenlijke vergassingsfase.
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