

# CHALMERS



## Thermodynamic process evaluation of a rotary kiln unit at LKAB Kiruna

*Master's Thesis within the Sustainable Energy Systems programme*

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Gothenburg, Sweden 2014



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**Cover:** Picture showing a rotary kiln unit at LKAB's mine site in Kiruna [1].

Chalmers Reproservice  
Gothenburg, Sweden 2014

## **Preface**

This public version of the Master Thesis “Thermodynamic process evaluation of a rotary kiln unit at LKAB” includes only parts of the total work performed. Due to the confidential requirements from LKAB, Chapter 4.4 is shortened and furthermore, the chapters about the validation of the model and the sensitivity analysis of the process are excluded.



## **Acknowledgement**

I would like to express my greatest appreciation to my main supervisor Assistant Professor Fredrik Normann for his guidance and support. Fredrik gave insightful comments and suggestions that helped me to find the right track especially at an early stage of my work. Furthermore, I am deeply grateful to my examiner Associate Professor Klas Andersson for providing me with such an interesting project and also for his guidance. The discussions with Fredrik and Klas had been very valuable.

Special thanks also to Johan Sandberg, my assistant supervisor at LKAB for his advice and information regarding the Grate-Kiln unit. I have greatly benefited from the visit to the facility at the Kiruna mine site and the numerous video conferences.

The experts at STEAG Energy Service GmbH deserve my gratitude for their extraordinary fast and professional answers and suggestions regarding the EBSILON professional software.

Finally, I also thank the entire team at the Department of Energy and Environment for the inspiring and instructive time.

Gothenburg, June 2014

Martin Haaf



## Abstract

This thesis describes the development of a thermodynamic model for the Grate-Kiln process. One application of such a process is the thermal treatment of iron ore pellets. The work has been performed in close collaboration with the iron ore producing company LKAB.

The model is applied to assess the process in terms of heat and mass flows. The thermodynamic assessment is carried out on an overall basis and for each of the three main process parts: grate, kiln and cooler.

The results reveal that the oxidation of the magnetite, contained in the inlet pellets, to hematite is the main heat source of the process. The heat release during the combustion of coal inside the kiln contributes to the remaining one third of the total heat supply. Half of the provided heat leaves the process as hot off gases. Thus, measures to improve the energy efficiency of the plant should focus on either reducing the mass flow of air that is heated by the process or making better use of the hot off gases.

In order to shift the models usability towards quantitative application, different measures could be taken. Among these, improvements in the data for validation, and enhancements in the modelling of the chemical properties of the iron ore pellets promise the greatest benefits.

**Key words:** *Iron ore pelletizing, Grate-Kiln process, Magnetite oxidation, Rotary kiln, Process modelling*



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## ABBREVIATIONS AND SYMBOLS

C	Cooler
C1	Cooler zone 1
C2	Cooler zone 2
C3	Cooler zone 3
C4	Cooler zone 4
DDD	Downdraft drying
G	Grate
K	Kiln
LKAB	Luossavaara-Kiirunavara Aktiebolag
PH	Preheating
TPH	Tempered preheating
UDD	Updraft drying

## Chemical formula

$\text{CaCO}_3$	Calcium carbonate
$\text{CaO}$	Calcium oxide
$\text{CO}_2$	Carbon dioxide
$\text{Fe}_2\text{O}_3$	Magnetite
$\text{Fe}_3\text{O}_4$	Hematite

## Latin Symbols

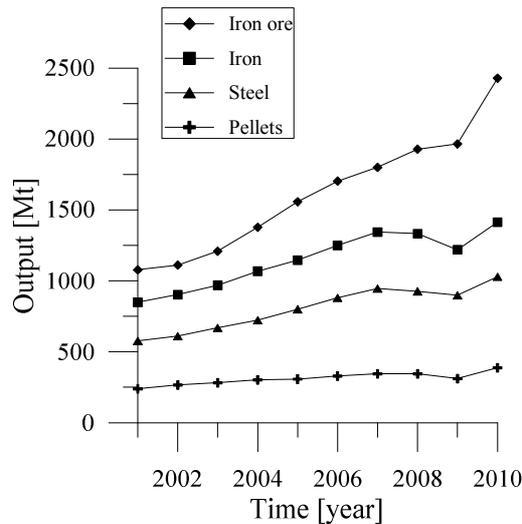
$c_p$	Specific heat	[J/kg*K]
$F_{\text{ox}}$	Fractional oxidation	[%]
$\Delta H_{\text{calc}}$	Heat of calcination	[J/mol]
$\Delta H_{\text{ox}}$	Heat of magnetite oxidation	[J/mol]
$\dot{Q}_{\text{rad}}$	Heat radiation	[W]
$T_g$	Temperature gas	[°C]
$T_p$	Temperature pellet	[°C]



# 1 Introduction

Iron and steel have played an important role in the technical development of modern civilisations. These materials are used in various fields of applications, such as construction, agriculture, generation and distribution of power, manufacturing of machinery and equipment.

The quantities of worldwide iron ore and iron ore based products during the years 2001 and 2010 are depicted in Figure 1-1. It reveals that the worldwide production of iron ore has been rising rapidly during the last decade. The amount of produced iron ore pellets was around 350 Mt in 2010. The trend in the increase of iron ore pellets consumption is predicted to continue [2] hence iron ore pellets will play an important role in the supply chain of raw material for iron and steelmaking processes.



**Figure 1-1** Global production of iron ore based products 2001 until 2010 [2]

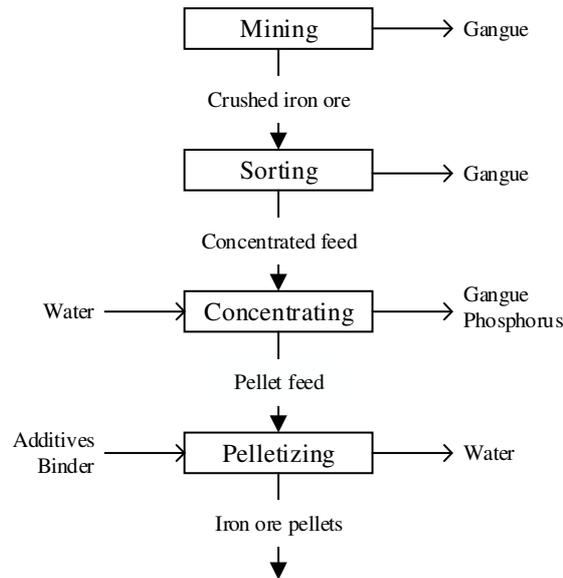
Besides fines, lumps and others, iron ore in the form of spherical pellets is used as a raw material for several primary iron and steelmaking processes. In comparison, the usage of pellets represents the following main advantages [3]:

- Ease of transportation
- Uniform granularity
- Improved gas permeability in the blast-furnace
- Increased furnace productivity

Luossavaara-Kiirunavara Aktiebolag (LKAB) is a producer of iron ore pellets. Their activities include all processing steps from mining the iron ore down in the ground to shipping of the final iron ore pellets. A brief overview about the processing chain and the relevant material flows that are involved in the production of iron ore pellets is given by Figure 1-2. The Grate-Kiln process which is part of the pelletizing and of great importance for this work, is further described in Chapter 2.

At first, the crude ore is mined by drilling or blasting at a depth of approximately 1000 m below sea level, in the world largest underground iron ore mine [4]. The ore is then conveyed via truck or train to crushers where it is coarsely crushed into smaller pieces. Afterwards, the chopped crude ore is hoisted up and transported to the sorting plant by means of conveyor belts.

In the sorting plant, the ground ore is further crushed and separated via various steps, basically consisting of grinding, sizing and magnetic separation. As an output, concentrated feed with an average grain diameter of 10 mm [5] leaves the plant.



**Figure 1-2** The process chain of iron ore pellets at LKAB Kiruna [6]

The concentrated feed contains considerable amounts of gangue and phosphorus which are removed in the concentration plant. Firstly, the concentrated feed undergoes various grinding and separation steps in order to reach higher iron content and reduced grain size. Afterwards, the phosphorus concentration is reduced by reverse flotation. The pellet feed slurry which is mainly consisting of iron ore and water is then transported to the pelletizing plant via pipes.

To obtain the required specific properties of the final pellets, additives are mixed with the pellet feed slurry in large tanks. After dewatering in rotating drums, the moisture content is reduced to 8.5 - 10 % [7], binder is added and the balling of the pellets is carried out. Some of the most common additives and binder materials are listed in Table 1-1, their usage depends on the requirements of the final pellets as well as on the compositions of the pellet feed. Following size separation, that guaranteed uniform size in the range of 10 to 12 mm [5], the wet green pellets enter the Grate-Kiln process for the final thermal treatment. Thereafter the pellets are ready for shipping.

**Table 1-1** Additives and binder materials used for the pelletizing [7]

Additives	Binder
Lime and lime-magnesium compounds	Bentonite
Recycling materials	Slaked lime
Ores with high bonding ability	Limestone
Quartz and quartzite	Dolomite

### Aim and Scope

This master thesis is part of the collaboration between LKAB and the Chalmers University of Technology. The overall focus of this work will be to contribute to the creation of new solutions for the energy efficient production of iron ore pellets in the

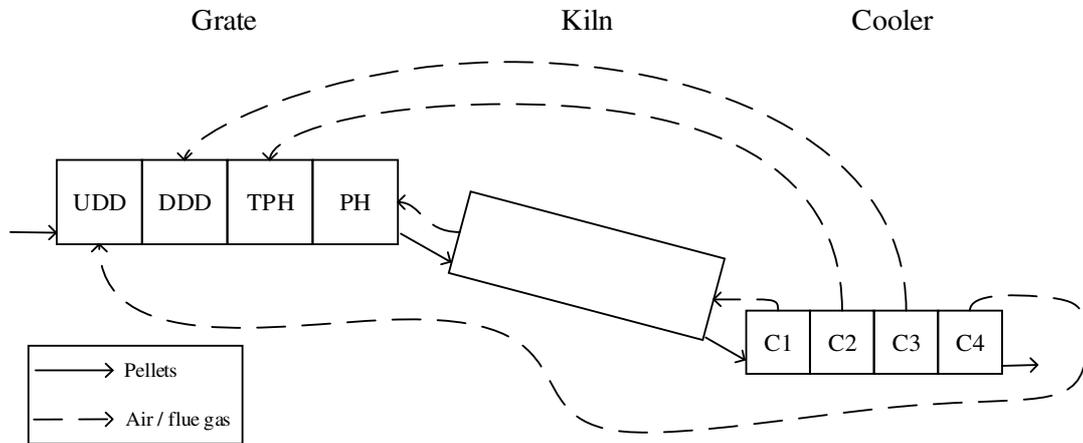
Grate-Kiln process, while at the same time achieving reduced CO<sub>2</sub> emissions. In today's Grate-Kiln process, coal is used as the primary fuel to reach the required temperature levels needed for a high quality and throughput of the iron ore pellet product. At the same time, a considerable amount of heat is supplied to the process via the oxidation of the iron ore itself. This process features result in a large excess of heat during the process, and in theory, the heat from the iron ore may be sufficient to run the process. The temperature level of the pellet bed is however critical to reach the required product quality and production rate. A considerable development work will be required to improve the use of the heat from the iron ore to reduce the input of primary fuel. This project aims to do a first assessment of the possibilities for improved energy utilization in the rotary kiln process.

The objective of the proposed project is to assess the heat and mass balances on an overall level in a rotary kiln unit at LKAB Kiruna. One important outcome of the thesis work will be the process simulation model that includes all thermal parts of the Grate-Kiln process. The work will contribute to the understanding of how heat and mass is transferred and transported in the unit.



## 2 The studied Grate-Kiln process

The thermal treatment of the green pellets is done within the Grate-Kiln process. The name Grate-Kiln refers to the first two process parts, namely the grate and the kiln. The cooler finally completes the process. A simplified schematic of that process, including the main material flows is provided in Figure 2-1.



**Figure 2-1** Schematic of the Grate-Kiln process at LKAB Kiruna [8]

The green pellets consist, as mentioned in Chapter 1, of several substances. Table 2-1 presents the compounds and each share. The main objective of the thermal treatment is the sintering of the pellets. As a side effect, the iron ore, which is mined in the chemical form of cubic magnetite, is oxidized to hexagonal hematite [9]. The magnetite oxidation releases considerable amounts of heat, which represents the main heat source of the process.

The sintering is needed to ensure a higher strength of the spherical pellets that makes them able to withstand the mechanical stresses during further handling. The hematite lattice with its higher stability contributes additionally to the increased mechanical strength of the final pellets. Another positive side effect is the increased reducibility of the hematite, compared with the virgin magnetite, in blast furnaces.

**Table 2-1** Average composition of the green pellets [10]

Compound	wt.-%
Magnetite	87.5
Silicon oxide	2.0
Calcium carbonate	1.0
Magnesium oxide	0.5
Moisture	9.0

In the four grate zones, the wet green pellets are preheated and dried by means of hot gases, which are injected either above or below the grate. Depending on the temperature level of the pellets, the main part of the magnetite oxidizes to hematite already on the grate. Inside the kiln, a rotating cylinder with a downwards slope, the pellets are sintered and further oxidized due to the higher temperature which is provided by the combustion of coal at the right end of the kiln counter current to the

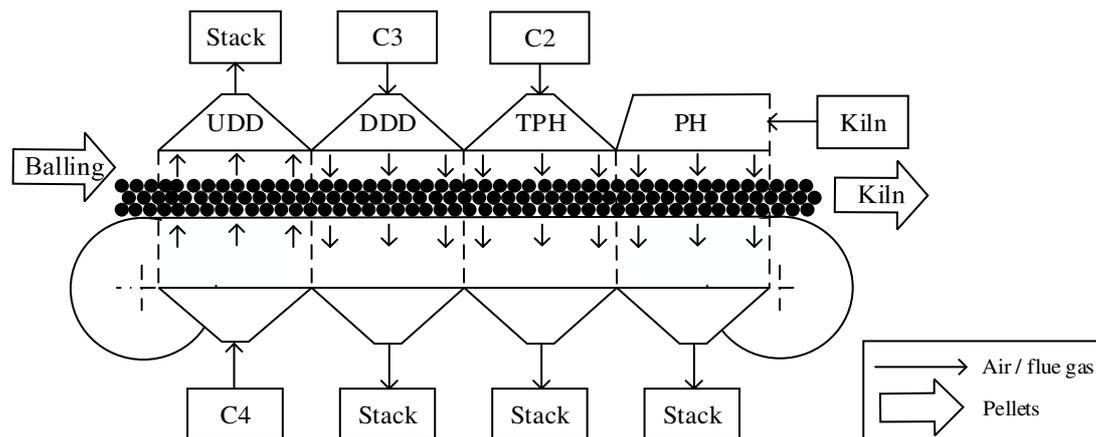
pellet flow. Great quantities of ambient air are used to cool down the pellets after the kiln inside the annular cooler. The resulting hot air streams are used for preheating and drying of the pellets on the grate. The main in- and outlets of the process are summarized in Table 2-2.

**Table 2-2** Main in- and outlets of the Grate-Kiln process

Inlet	Outlet
<i>Green pellets (~90 wt.% magnetite)</i>	<i>Final pellets (~95 wt.% hematite)</i>
<i>Ambient air</i>	<i>Air / flue gas</i>
<i>Fuel</i>	

## 2.1 Grate

The grate itself is the largest part of the Grate-Kiln unit with a total length of 53 m and a width of 4.5 m. It is separated into four zones. It starts with the updraft drying (UDD) zone, where hot air is blown in from below the pellet bed. In the downdraft drying (DDD) zone and the tempered preheating (TPH) zone, the air is blown in downwards from above the pellet bed. Flue gas out of the kiln heats up the pellets in the preheating (PH) zone. A schematic of the grate is provided in Figure 2-2.



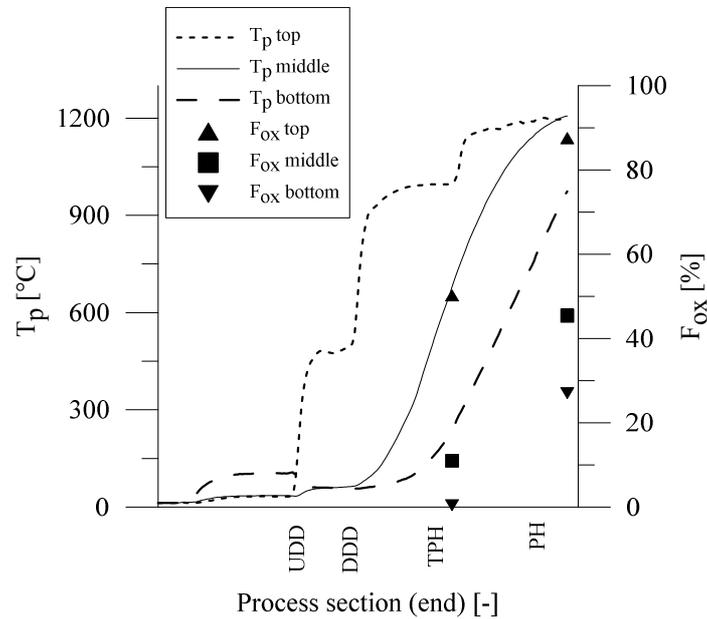
**Figure 2-2** Schematic of the Grate-Kiln grate and its zones

At the beginning of the grate, the wet green pellets from the balling procedure are evenly distributed on the grate with a height of max. 23 cm. If this limit is exceeded, the pellets in the lower bed regions could be crushed, since they cannot bear the load of the upper pellets layer. During the four grate zones, the pellet bed is completely dried and further heated. Within the TPH and the PH zone, the main part of the magnetite is oxidized to hematite.

Inside the pellet bed on the grate, the temperature differences over the height are quite significant. Figure 2-3 shows, the temperature profile of the pellet bed during its progress on the grate and the resulting fractional oxidation of the pellets after the TPH and PH zone respectively. Both data sets are based on a measurement campaign from the Grate-Kiln unit [11].

During the UDD zone, hot air from C4 is blown in from below the grate, therefore the temperature of the bottom layer records highest increase. Water starts to evaporate in the bottom layer, whereupon it condenses in the upper layer due to prevailing low temperatures. Within the following three zones, the hot gases are supplied from above

the grate to prevent the grate steel materials from being damaged by excessively high temperatures. The remaining moisture is evaporated and the pellet bed is further heated. In the DDD zone, the average bed temperature is increased to around 150 °C, whereas it reaches 670 °C and 1150 °C in the TPH and the PH zone respectively.

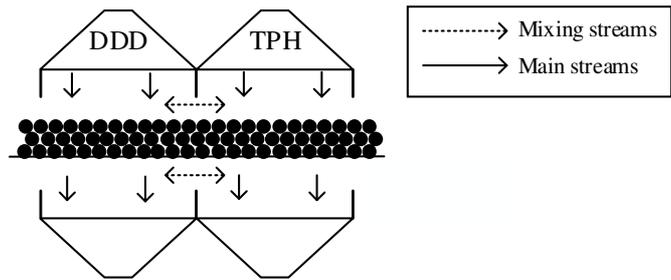


**Figure 2-3** Continuous temperatures profile and the resulting fractional oxidation levels of the pellets after the TPH and PH zone on the grate

Since the pellet temperature is one of the main driving forces for the magnetite oxidation, the differences in the fractional oxidation of the pellets over the bed height differs equally to the pellet temperature. As shown in Figure 2-3, the oxidation starts during the TPH zone and the fractional oxidation is further increased during the PH zone. At the interface between grate and kiln, the average oxidation is somewhere around 60 %, whereas the absolute difference between top and bottom layer could reach 60 % as well.

Besides other factors depending on the pellet composition and the resulting chemical properties, the initial temperature of the hot gases is of great importance for the pellet strength. The heat supply has to be controlled so that the arising water vapour and the air inclusions still existing in the pores can escape or expand from the pellet core through the capillaries without any ensuing over-pressure [7]. Especially in the UDD and to some extent in the DDD zone, the temperature of the hot gases needs to be lowered. This lowering is ensured via ambient air that could be blended to the hot air streams between cooler and grate in order to reduce the resulting air temperature. The maximum temperature level for the hot gases is around 140 °C for the UDD and 420 °C for the DDD zone.

Above and below the grate and the cooler, a mixing of gas streams could occur. This phenomenon is based on the fact that the panels between the zones are not able to separate the main gas streams with it's different pressure conditions completely. Figure 2-4 depicts the situation between the DDD and the TPH zone.



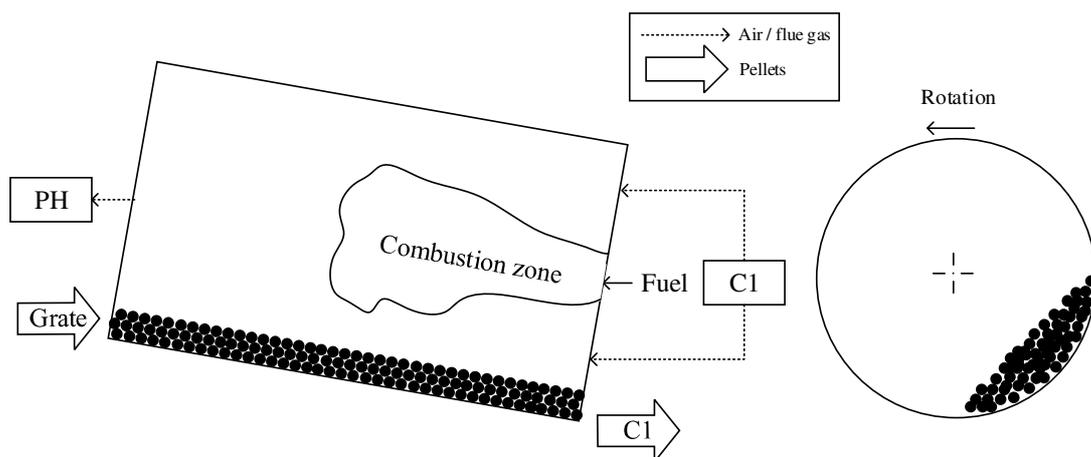
**Figure 2-4** Schematic of the gas mixing phenomena between the DDD and the TPH zone

As mentioned above, the Grate-Kiln unit is operating below ambient pressure. Due to this, air from inside the facility hall is drawn into the process at several positions. This causes temperature reductions at the affected sections. Especially at the interface between PH zone - Kiln and Kiln - C1, the aspirated leakage air flows and hence the reductions in gas temperatures are quite substantial. As pointed out before, the pellet temperature is one of the most important parameters for the kinetics of the magnetite oxidation, and hence the release of the oxidation heat. Since the pellet temperature is strongly affected by the temperature of the corresponding gas stream, it is crucial to be aware of the leakage air streams.

The leakage mass flows at the beginning and at the end of the grate are the largest. However, the leakage into the PH zone is the more important one. Compared to the other zones, the mixing between the TPH and the PH zone is quite significant due to the fact that the hot flue gas from the kiln is blown in horizontally.

## 2.2 Kiln

The kiln is a rotating cylinder with an average inner diameter of 5 m and a total length of 33.5 m. A schematic of the kiln is illustrated in Figure 2-5. To achieve a further temperature increase of the pellets, coal is combusted counter current to the pellets flow. Due to the high mass flow of air that is blown in from C1, the corresponding stoichiometric ratio of the combustion is around 5 to 6. At the Grate-Kiln unit, coal is used as the primary fuel, but it is also possible to use oil instead. Under standard process conditions, the heat input by the fuel is in the range of 30 and 40 MW.



**Figure 2-5** Schematic of the Grate-Kiln kiln

The heat transfer inside the kiln is complex. Heat radiation between flame, particles, inner kiln surface and pellets is the predominating heat transfer type constituting over 90 % to the total heat transferred to the pellets [12]. The length of the flame

determines the radiative heat transfer distribution over the kiln length. To avoid temperature peaks inside the kiln, and hence a highly uneven axial temperature profile a long flame is desired. In addition to the heat radiation, heat is transferred via convective heat transfer between the flue gases, pellets and inner kiln surface.

The combustion ensures the increase of the pellet temperature to around 1200 to 1300 °C. These high temperatures are needed to force the sintering of the pellets that guarantees additional mechanical strength [13]. Besides the sintering, the fractional oxidation of the pellets is further increased. Because of the rotation of the kiln, the pellets are evenly mixed and the temperature differences are quite low compared to the grate. Thus, the fractional oxidation of the pellets at the end of the kiln is more uniform. Owing to the high pellet temperature, some dissociation of the hematite back to secondary magnetite could occur [14], [15].

The radiative heat losses from the outer kiln surface are another important heat sink. Calculations were performed by LKAB regarding the heat transfer through the kiln shell and the resulting radiative heat losses at the outer kiln surface. They came up with a total radiation loss of approximately 4.3 MW [10]. The calculations are based on the model assumptions of a radiating hot cylindrical body with a length of 34 m, an average outer diameter of 5.75 m and a surface temperature of 250 °C.

### 2.3 Cooler

The last part of the Grate-Kiln process is the cooler. As shown in Figure 2-6, it is designed as a rotating angular ring, with a mean diameter of 16 m and an average width of 3 m.

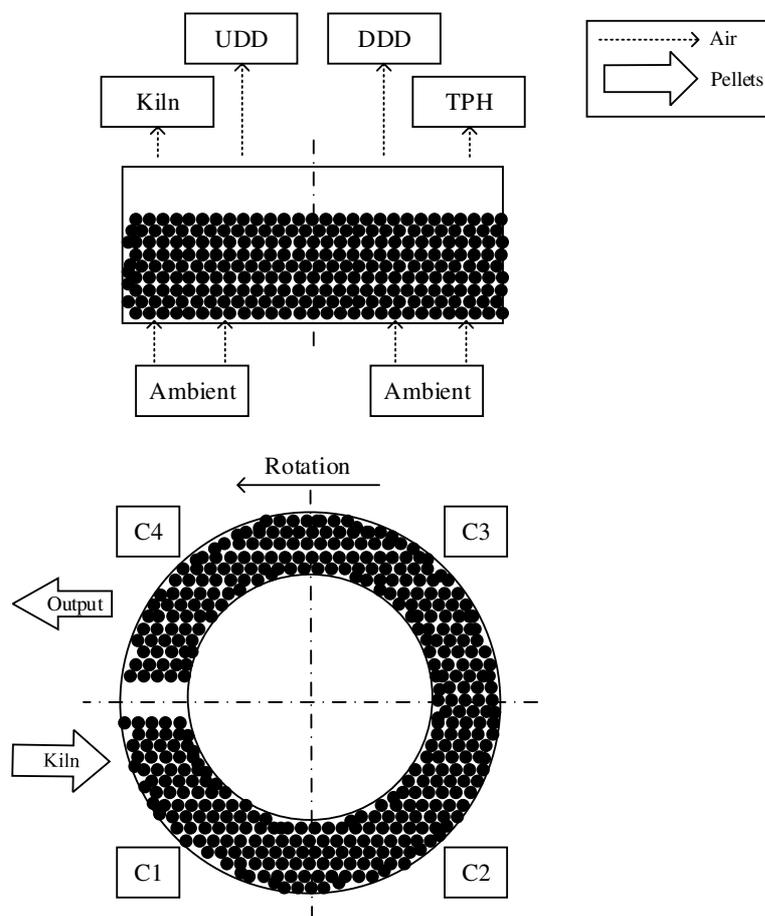


Figure 2-6 Schematic of the Grate-Kiln cooler

In order to cool the pellets down to around 100 °C, ambient air is blown in from below. Leakage and mixing of air streams, as described in Chapter 2.1, also occur within the cooler. The cooler is divided into four zones. The air heated by zone C1 supplies the kiln with hot air, whereas the heated air streams out of zone C2 to C4 are directly led to the grate. In the cooler zones C1 and C2, the pellet temperature could still be above 1000 °C hence the fractional oxidation of the pellets is further increased. Due to the induration of the pellets achieved, the bed height inside the cooler is increased to around 1.6 m.

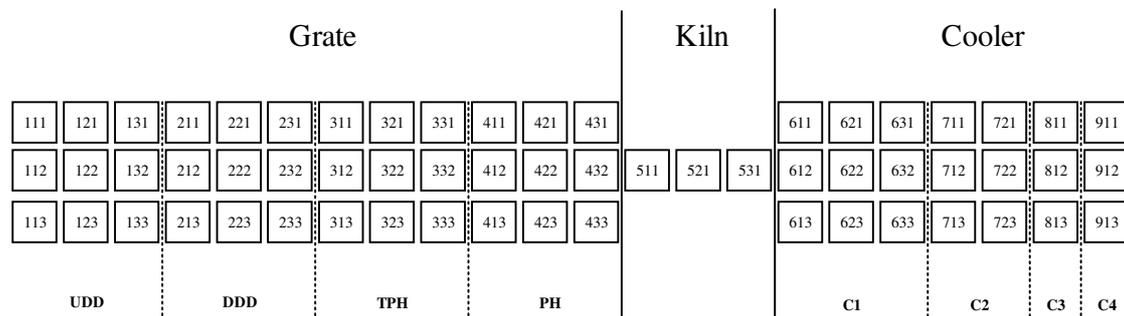
### 3 Method

The work is based on a literature review to obtain the necessary expertise and the knowledge to understand the functioning of the Grate-Kiln unit. The review is twofold, process relevant documents from LKAB referring to the Grate-Kiln unit and its features needs to be considered as well as other scientific sources regarding processing of iron ore pellets and rotary kiln technology. Followed by identifying and gathering of the required process data from the existing Grate-Kiln unit, a thermodynamic model is developed.

During the entire work, a close collaboration with LKAB is required to obtain the appropriate information in terms of process control, design and flow conditions of the Grate-Kiln unit.

EBSILON Professional 10.0 is used for modelling purposes. This software is typically applied for heat and mass balance calculations of large thermal systems such as power plants and other industrial thermal systems. Programmable elements are implemented to model the thermodynamic influences of the important chemical reactions, since the possibilities to embed such with the available components are limited. The model is designed to describe the thermal aspects of the process in case of steady state conditions. Any electricity demands for pumps, fans and other engines are not considered.

The model structure is derived from the structure of the Grate-Kiln process. The three main parts, namely grate, kiln and cooler are divided into subsystems according to Figure 3-1.



**Figure 3-1** Overview about the structure of the model and the introduced subsystems

The pellet temperature is the main factor that influences the reaction rate of the magnetite oxidation. The heat released by the oxidation is, furthermore, the main heat source of the whole process. Within the pellets bed on the grate as well as on the cooler, the temperature gradients are quite significant. To enable the model to take the temperature gradients into account, the whole pellet stream is divided into three layers. On the grate, the middle layer consists of 60 % of the whole pellet mass flow, whereas the top and the bottom layer covers 20 % respectively.

To describe the progress of the pellets within every section, three subsystems per layer are introduced. Due to the mixing of the pellets inside the kiln, the temperature profile is assumed to be uniform hence the complete pellet stream is treated as one layer. Since heat transfer is the only phenomenon that occurs within C4, C3 and the second part of C2, the number of implemented sub-systems in these process sections is reduced.

Every sub-system got its own number that describes its position inside the model. The first digit shows the process section within the Grate-Kiln process according to Table 3-1. The second digit indicates the progress within one section. The layer is pointed out by the last digit. To sum up, the whole model consists of 60 connected sub-systems. Each sub-system is implemented as a macro object with several included sub-routines.

**Table 3-1** Numbering and distribution of the implemented subsystems

<b>Part</b>	<i>Grate</i>				<i>Kiln</i>	<i>Cooler</i>			
	<i>UDD</i>	<i>DDD</i>	<i>TPH</i>	<i>PH</i>	<i>Kiln</i>	<i>C1</i>	<i>C2</i>	<i>C3</i>	<i>C4</i>
<b>Section</b>									
<b>Number</b>	1	2	3	4	5	6	7	8	9

The model characteristics could be summarized as a two-dimensional approach that considers different process residences of the pellets, and in addition to that, different layers within the pellets bed on the grate and on the cooler. Any parameter changes over the bed width are not considered.

## 4 Modelling

The main objective of this work is the development of a thermodynamic model that provides information in terms of heat and mass flows on an overall basis within the Grate-Kiln process. In order to do this, it is crucial to keep the right balance between the depth of detail needed to describe the ongoing phenomena sufficiently and the complexity of the whole model.

The implementation of the iron ore pellet stream in the model is presented in Chapter 4.1. The modelling of the considered chemical reactions is described in Chapter 4.2 and the corresponding subroutines are explained in Appendix A. Chapter 4.3 delivers specific information regarding the modelling of each of the three process parts. Due to the fact that not every parameter needed as an input variable for the model is measured in the Grate-Kiln unit, some data must be assumed for the first time. Chapter 4.4 gives a categorization of the necessary input data depending on whether they are well-defined or assumed.

### 4.1 Iron ore pellets

To be able to describe the wet iron ore pellets in the model, the stream is divided into a dry green pellet and a water stream. The dry green pellet flow is treated as a user-defined fluid, described by its  $c_p$ -coefficients. It is considered as a mixture between magnetite and hematite.

Figure 4-1 shows the specific heat both for the magnetite and the hematite phase within a temperature range from 300 to 1600 K. It is obvious that the  $c_p$ -values vary over the considered temperature range. Especially between 800 and 1000 K the changes are quite significant.

In the model a constant  $c_p$ -value of 0.88 kJ/kg\*K is assumed. The choice of this value is based on two facts. In the critical process sections pellet temperatures above 1000 K are predominating. In this temperature range the chosen value is quite accurate. Furthermore, the deviation below 1000 K will level out at an overall basis. To sum up, a constant  $c_p$ -value causes some inaccuracies, but for the important temperature ranges as well as on an overall basis, the inaccuracies are negligible.

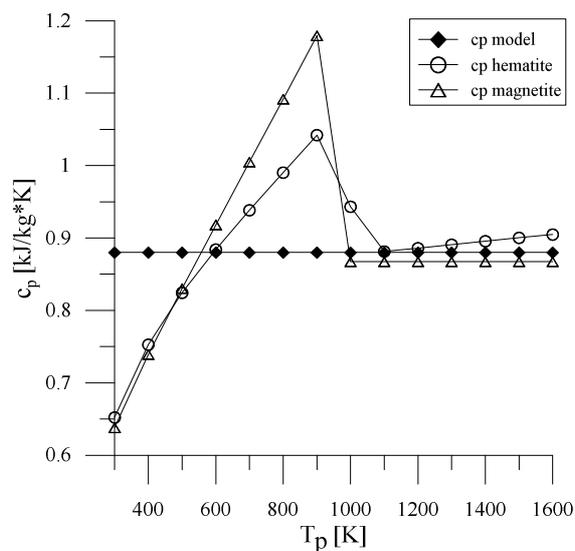


Figure 4-1 Specific heat for magnetite, hematite and the one used in the model [16]

## 4.2 Chemical reaction modelling

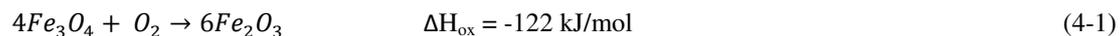
During the entire Grate-Kiln process, several chemical and metallurgical reactions are taking place, depending on the pellet composition and its compounds. The reactions overlap and influence each other. Some of them are listed below [17]:

- Calcination of calcium carbonate
- Oxidation of magnetite
- Reaction between calcium oxide and hematite
- Dissociation of hematite

With regard to the performed heat balance, the exothermic oxidation of magnetite and the endothermic calcination of calcium carbonate are of great concern. The considered influence of both reactions and their implementation in the model is further explained in the following chapters.

### 4.2.1 Oxidation of magnetite

A positive side effect of the thermal treatment of the pellets is the oxidation of magnetite to hematite, as shown in equation 4-1. Depending on the total mass flow of the green pellets, the corresponding magnetite content and finally, the fractional oxidation of the pellets after the cooler, the total heat release at the Grate-Kiln unit ranges between 65 to 75 MW. The amount of released heat shows the importance of the implementation of the reaction.

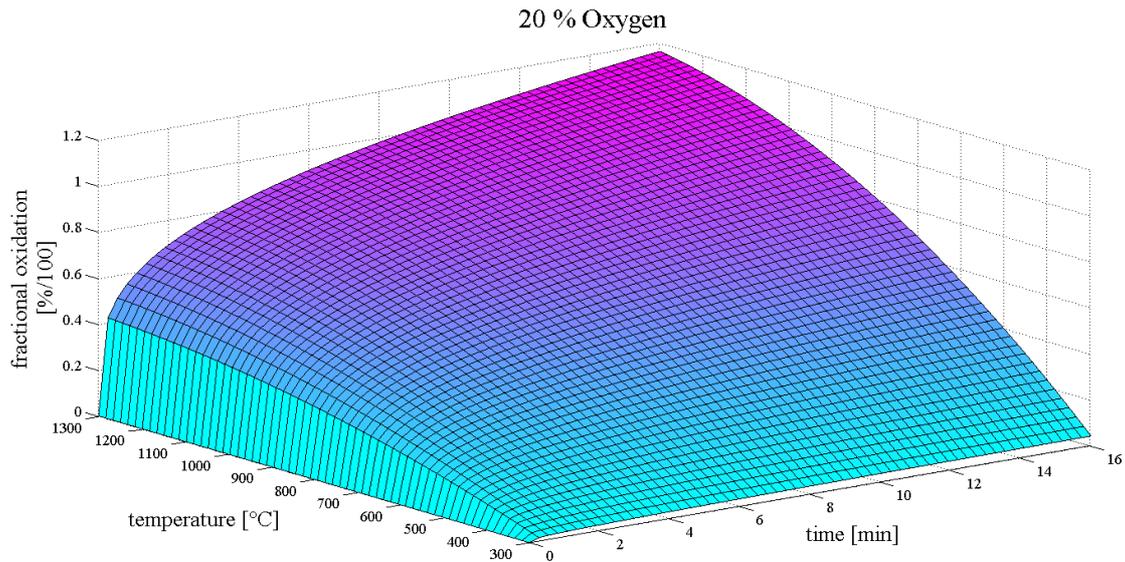


The following factors that influence the magnetite oxidation are considered in the model:

- Pellet temperature
- Oxygen concentration of the surrounding gas
- Fractional oxidation of the pellet

The measurements provided by Liang and Yang [18] are used for the approximation of the equation for the description of the reaction kinetics, depending on the above mentioned factors, that are applied in the model. Figure 4-2 shows a magnetite oxidation curve for 20 % oxygen concentration in the surrounding gas. Similar curves for 15, 10 and finally 5 % oxygen concentration are provided in Appendix C.

In addition to the enthalpy changes of the pellet stream caused by the heat release, the oxygen reduction in the involved gas stream is considered. As pointed out above, the oxygen concentration is one of the driving forces for the magnetite oxidation, therefore it is crucial to consider such changes. The increase in the pellet mass flow caused by the bounding of the oxygen is neglected.



**Figure 4-2** Fractional magnetite oxidation depending on pellet temperature and roasting time for 20 % oxygen in the surrounding gas

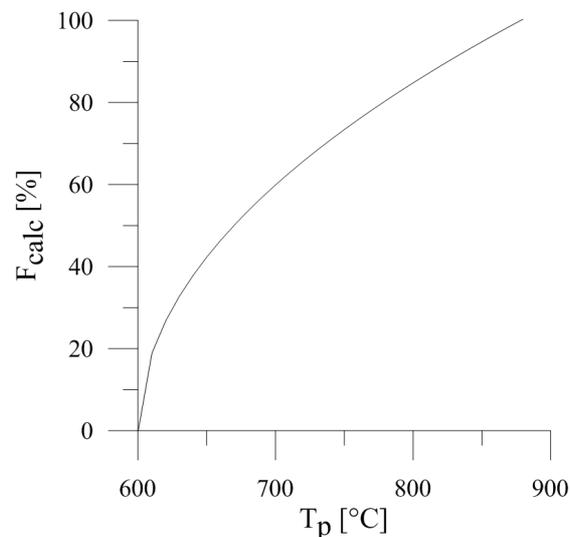
## 4.2.2 Calcination of calcium carbonate

Besides the oxidation of the magnetite as a heat source, the endothermic calcination of calcium carbonate to calcium oxide according to equation 4-2 is considered as well.



The calcium carbonate content in the green pellets varies between 1.0 to 2.0 %, hence the total heat consumed by this reaction could be determined to the range of 4 to 8 MW. Due to the fact that this heat demand represents only ~8 % of the total heat that is supplied to the process, the function of the calcination reaction kinetics takes only the pellet temperature into account. The implemented equation delivers the calcination curve as shown in Figure 4-3.

It is assumed that the calcination starts at 600 °C and a full conversion is achieved at 900 °C [19]. In the model, the enthalpy reduction in the involved pellet stream represents the only influence that is considered.



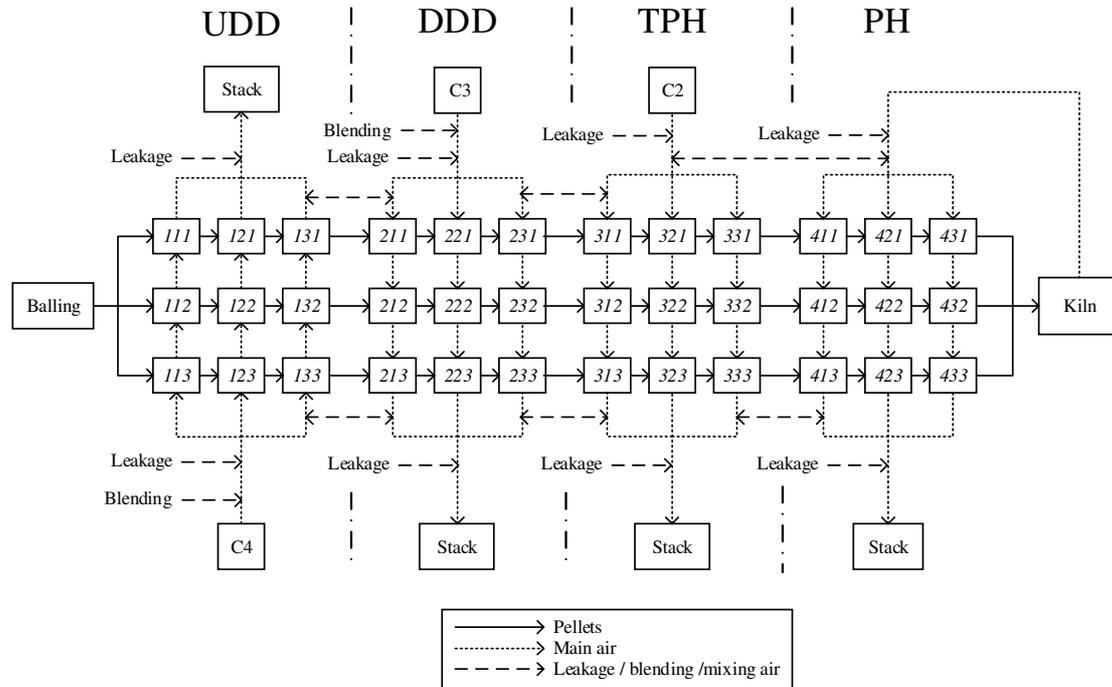
**Figure 4-3** Fractional calcination depending on pellet temperature

## 4.3 Modelling of the process parts

The following paragraphs provide an overview of the model structure for each process part and the implementation of the interactions between the involved streams.

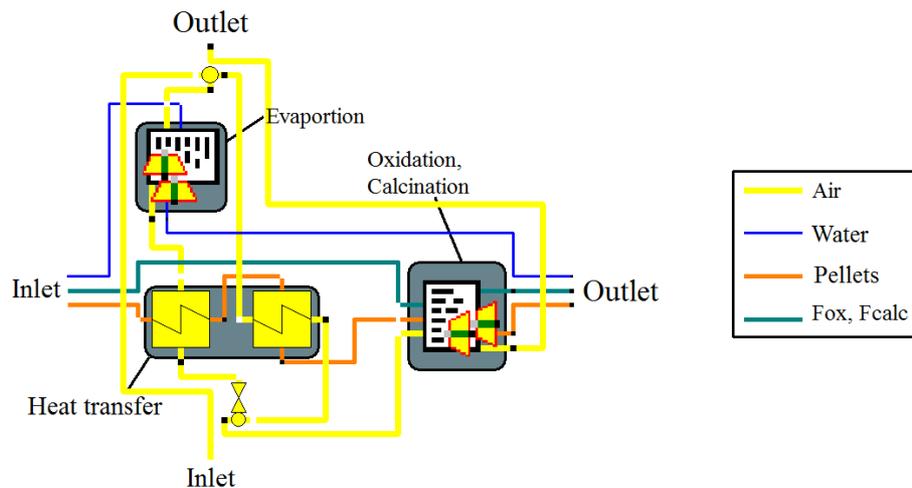
### 4.3.1 Grate

The schematic of the grate model is depicted in Figure 4-4. It includes all considered mixing and leakage streams as well as the position of the optionally blending streams.



**Figure 4-4** Schematic of the grate model structure, including the subsystems as well as the considered pellet and gas streams

48 sub-systems are used for the grate modelling. The characteristic of each partition is calculated with a macro. Figure 4-5 depicts one of the macros used within the first three grate zones. In the PH zone, the air stream is replaced by a flue gas stream.



**Figure 4-5** Illustration of the macro used for the grate

The pellet stream enters the macro on the left hand side. If the temperature of the air stream is higher than the pellet stream temperature, the air enters the evaporation

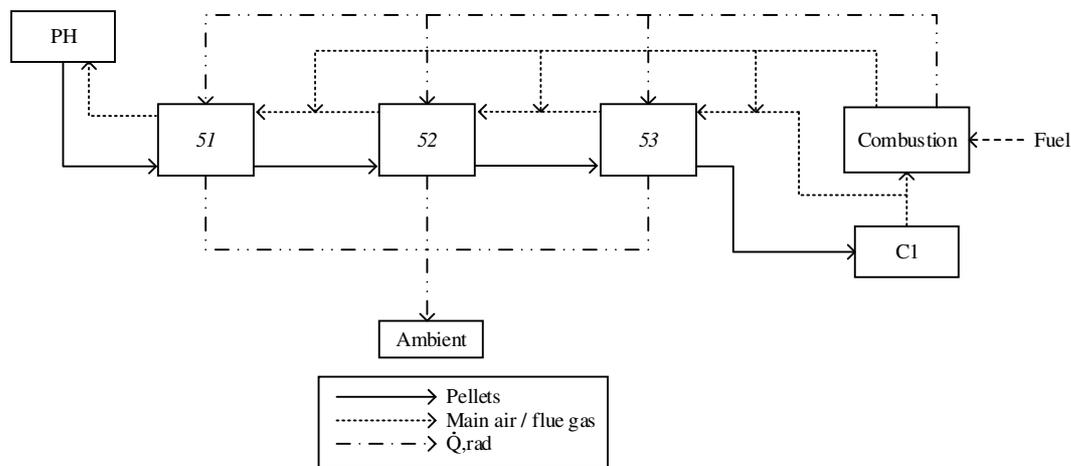
component. Within that component, the heat loss caused by the evaporation of the water is modelled according to the subroutine which is explained in Appendix A. Further on, the mass flow of the outgoing water is reduced by the amount of the evaporated water. Afterwards, the remaining temperature difference is used for heating up the pellets.

If the air stream temperature is lower than the pellet stream temperature, the other air stream path is chosen and the air stream is heated up by the pellet stream. Due to the intensive contact between the pellets and the air within the pellet bed, the efficiency of both involved heat exchangers is set to 95 %.

After heat transfer and evaporation, the pellet stream enters the oxidation and calcination component. The involved subroutines are described in Appendix A. The component sets the new the fractional oxidation and the new enthalpy of the pellet stream. Further on, the oxygen content of the air flow is reduced by the amount of oxygen that is bounded due to the magnetite oxidation.

### 4.3.2 Kiln

The kiln is the most crucial part within the Grate-Kiln process. A schematic overview of the kiln model including the relevant material and heat flows is given in Figure 4-6. Due to the mixing of the pellet stream caused by the rotation of the kiln cylinder, a regular radial temperature profile is assumed. Hence, compared to the grate, only one single pellet stream consisting of pellets with three different fractional oxidation levels, as transmitted from the grate, goes through the kiln model. Thus, in total three macros are used to describe the pellet related phenomena inside the kiln.

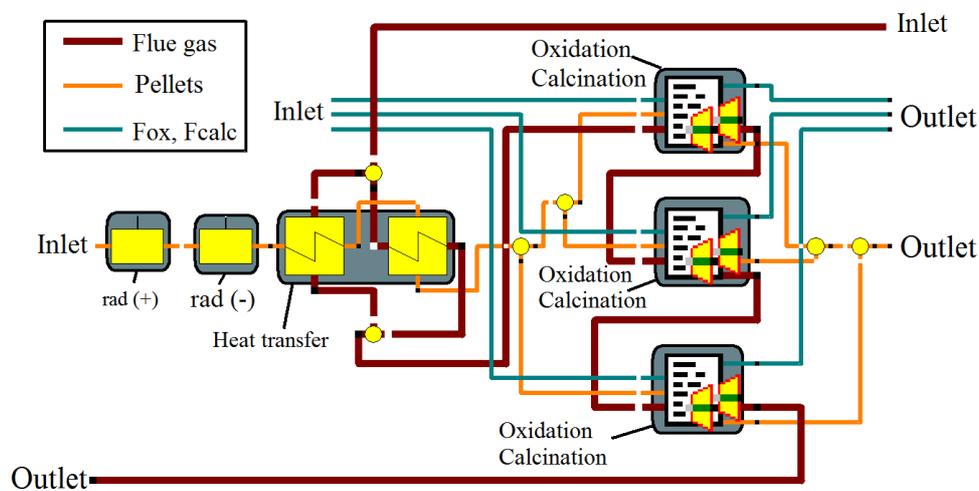


**Figure 4-6** Schematic of the kiln model structure including the subsystems and the modelled material/heat flows

Within the kiln, the adequate modelling of the combustion and the resulting heat transfer is essential. For this purpose, a combustion chamber with heat output (component 21) is used in EBSILON. The fed combustion air consists of hot air out of C1 and a certain amount of leakage air that is drawn in between C1 and the kiln. This air stream is split before it enters the combustion chamber. The amount of air that is involved in the combustion is set to be 50 % of the total air that enters the kiln. After the combustion there is a cold air stream close to the inner kiln surface and a hot flue gas stream in the kiln centre. Ahead of each kiln macro one third of the inner hot flue gas stream is mixed together with the outer cold air stream hence a linear gas mixing over the kiln length is assumed and implemented.

The difference between the total heat input, defined by the fuel mass flow and its corresponding net caloric value, and the heat that is consumed for heating up the incoming air to the set flue gas temperature, is defined to be the heat that is transferred via heat radiation. This radiation heat is distributed to each of the kiln macros. By changing the radiation heat distribution, different flame lengths could be observed. The radiative heat losses are considered to be equal over the whole kiln length. Therefore, one third of the total radiation loss is directly reduced from each of the involved macros.

Depending on their height within the pellet bed on the grate, the fractional oxidation of the pellets differs, as shown in Chapter 2.1. To maintain these varieties in terms of fractional oxidation, it is assumed that the main pellet stream consists of pellets with three different fractional oxidation levels. Therefore, three oxidation lines and consequently three oxidation / calcination components are needed for each kiln macro. The resulting macro is illustrated in Figure 4-7.



**Figure 4-7** Illustration of the macro used for the kiln

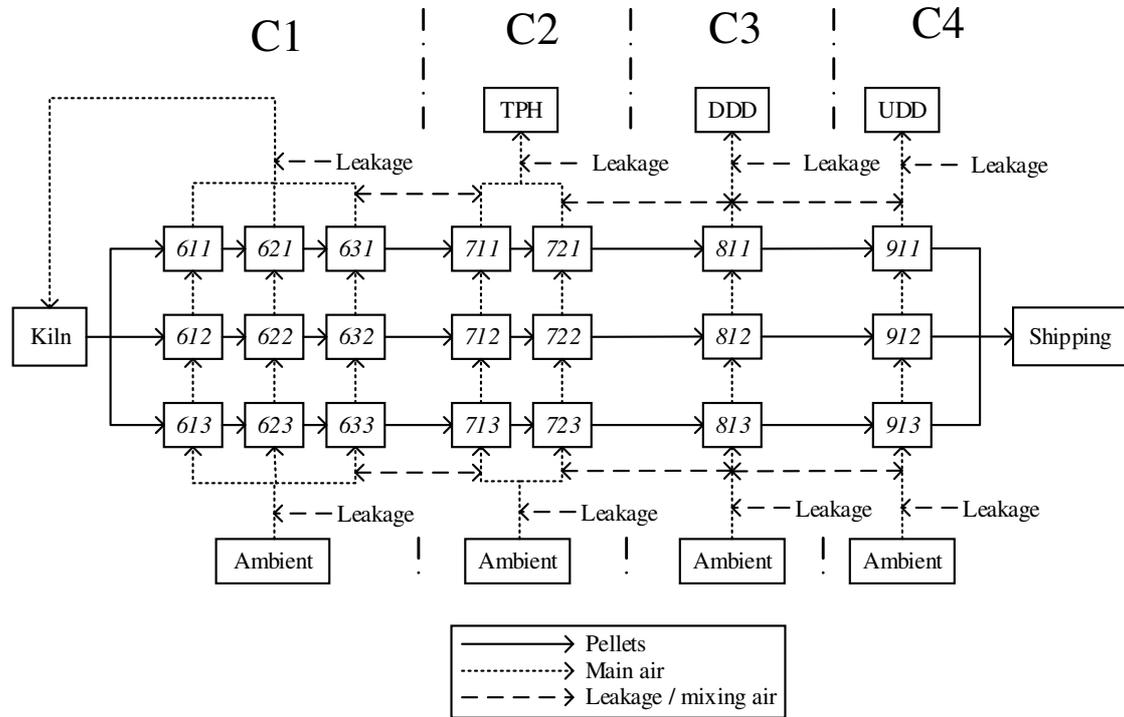
The pellet stream enters the macro on the left hand side. First, the radiation heat from the flame is added to the pellet stream (component 16) followed by the extraction of the heat that is caused by the radiative heat losses (component 15). Afterwards, similar to the grate macro, heat is transferred between flue gas and pellets, the direction of this heat transfer depends on the predominant temperature levels of the streams. In case of the kiln, the conditions for the convective heat transfer between pellets and flue gases are poor and therefore the heat exchanger efficiency set to 10 %.

After the heat transfer, the pellets stream is split with the same mass flow ratio as on the grate (20 % - 60 % - 20 %). Each part pellet stream entering its own oxidation / calcination component. At this point, again the reference to the Appendix A which exemplifies both subroutines used. The flue gas stream that delivers the actual oxygen concentration which is needed for the oxidation subroutine goes sequentially through all of the oxidation / calcination components. Finally, the pellets are mixed together again.

### 4.3.3 Cooler

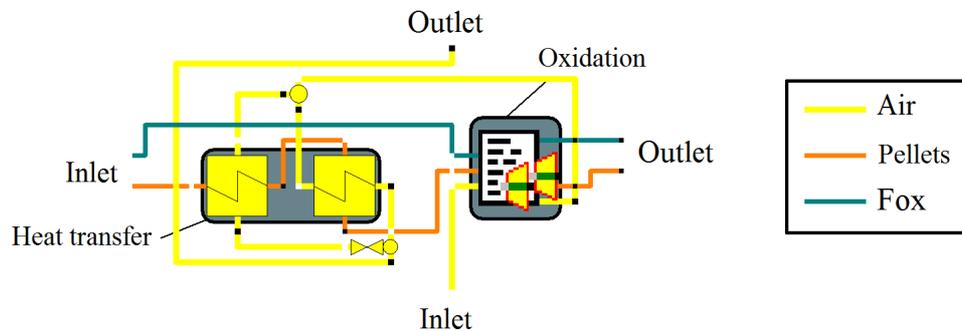
The model structure of the cooler is similar to the grate's one. A schematic is depicted in Figure 4-8. However, the number of macros per layer is different. The choice is again based on the overall ambition to describe the ongoing phenomena sufficiently. In the first two cooler zones, where the temperature of the pellets - especially within

the top and middle layers - could still be high and hence the magnetite oxidation proceeds, three, respectively two subsystems per layer are applied. Within C3 and C4 there is mainly heat transfer between pellets and air occurring, hence one subsystem per zone is adequate.



**Figure 4-8** Schematic of the structure of the cooler model including the subsystems and the considered pellet and air streams

The macro used for the cooler modelling is shown in Figure 4-9. It starts with the heat transfer between pellets and air followed by the magnetite oxidation component. The calcination is assumed to be completed within the kiln, thus it is not implemented in the cooler macros. According to the previous macros, the direction of the heat transfer depends on the temperature of the involved streams. Due to the intensive contact between the pellets and the air within the pellets bed, the efficiency of both heat exchangers involved is set to 95 %, similar to the grate's heat exchangers efficiency.



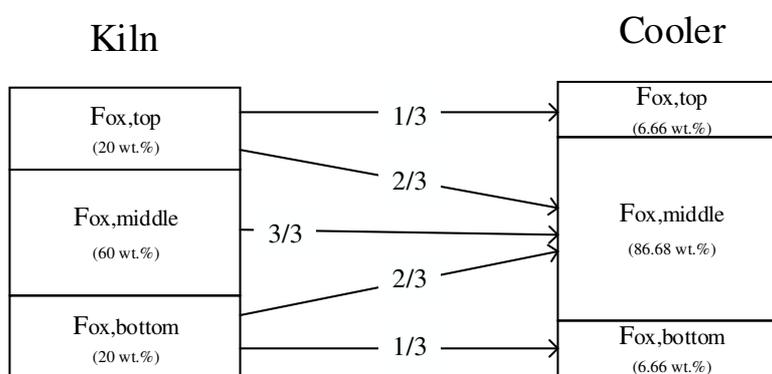
**Figure 4-9** Illustration of the macro used for the cooler

Within the kiln, the temperature of the pellet streams is assumed to be equal, in contrast to that, the three fractional oxidation levels transmitted from the grate are still treated differently. Thus, at the interface between kiln and cooler, one single pellet

stream consisting of pellets with three different fractional oxidation levels needs to be distinguished into the three cooler layers.

Theoretically, one third of each sub stream out of the kiln is fed to each cooler layer. The modelling of this circumstance will result in three different fractional oxidation levels per layer and in total nine different fractional oxidation levels that need to be described within the cooler.

In order to keep the model understandable, the approach demonstrated in Figure 4-10 is chosen. The generic ambition is to show the extremes in terms of fractional oxidation levels that could occur in the final pellet product after the process. The highest fractional oxidation level reaches the sub stream from the top layer of the grate that is fed to the top layer within the cooler. Similar to that, the lowest fractional oxidation level experiences the sub stream from the bottom of the grate that is fed to the bottom layer of the cooler.



**Figure 4-10** Schematic of the mass distribution of the pellet stream between kiln and cooler

As a summary, in the model, the cooler top layer consists of one third of the grate's top layer. Simultaneously, the cooler bottom layer consists of one third of the grate's bottom layer. The remaining sub streams are mixed together and the resulting fractional oxidation is calculated according to each mass portion.

## 4.4 Input data

Process data from the Grate-Kiln unit are used as input to the modelling. Most of the process parameters change during the year depending on several factors like variations in the properties of the mined iron ore or in the ambient air temperature. In order to cope with the parameter changes within the process, one reference case is defined. All the input data are based on the reference case. The input data are considered as two different categories:

- Well defined
- Assumed

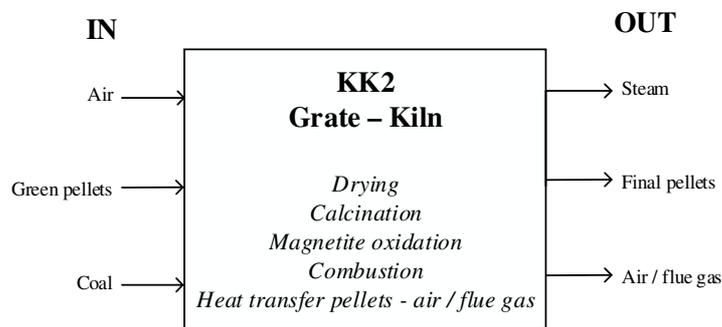
With regard to the assumed parameters, the following approach was used. In the beginning, a range for each value is defined, based either on measurement data that could be used for deriving such a range or on estimations from LKAB. Afterwards, the model is fed with the assumed value within that range. By performing several iterative modelling runs the final value is determined in order to minimize the difference between the modelling results and the reference case data.

## 5 Mass and heat balances

Chapter 5.1 provides mass and heat balances for the Grate-Kiln process. Further on, the same kind of overview is presented for each of the three process parts (chapters 5.2 - 5.4). The involved mass and heat flows are listed and further described. All numbers are based on the defined reference case. Detailed tables are provided in Appendix D.

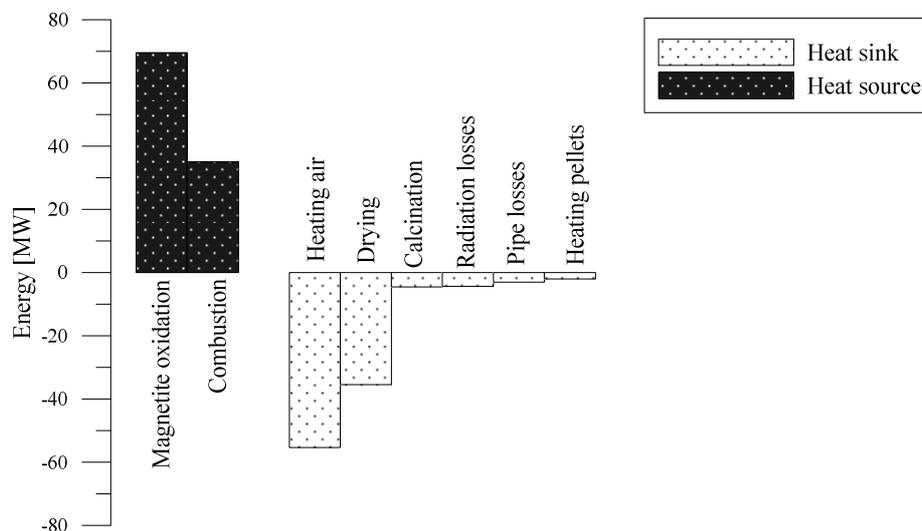
### 5.1 Process overview

Figure 5-1 gives an overview of the material flows as well as the considered phenomena inside the Grate-Kiln unit. During the process the wet green pellets are dried almost the entire magnetite oxidized to hematite and the calcium carbonate is converted to calcium oxide. To achieve the needed pellet temperatures for sintering, coal is combusted inside the kiln.



**Figure 5-1** Thermodynamic overview about the Grate-Kiln process

Summing up, the heat effects caused by the involved material flows, the chemical reactions as well as the considered heat losses, all heat sources and heat sinks are determined and shown in Figure 5-2.



**Figure 5-2** Heat sources and heat sinks of the Grate-Kiln process

In the Grate-Kiln process around 100 MW are transferred between heat sinks and heat source. The main heat source is the oxidation of the magnetite (66 %). The dominating sinks are the heating of ambient air (52 %) followed by the drying of the green pellets (34 %). It could be observed that the considered radiation (4.1 %) and

pipe (2.8 %) losses as well as the calcination of the calcium carbonate (4.3 %) are insignificant heat sinks at the overall level.

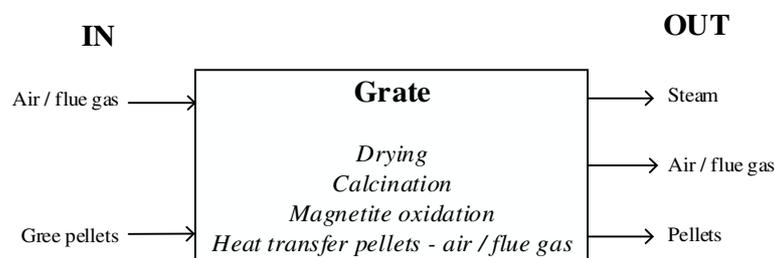
A first measure to improve the process efficiency could be the tackling of the hot off gases. In order to do so, either the amount of air that is heated up by the process needs to be decreased or the utilization of the heat contained in the off gases must be improved.

The total mass flow of the off gases (~400 kg/s) consists of main air (66 %), leakage air (13 %) and blending air (21 %). The latter is determined by the maximum initial temperature of the hot gases as they enter the grate and therefore are not reducible without worsening the quality of the pellets (Chapter 2.1). The amount of main air is needed to cool down the pellets inside the cooler and simultaneously for heating up the pellets on the grate. Thus, reducing the mass flow of one of the four main streams will result in a temperature increase of the pellets after the cooler as well as in a decrease of the supplied heat to the grate. Hence, the process efficiency will decrease. The last portion of the hot off gases is the leakage air. Such streams do not contribute anything to pellets` quality and are therefore dispensable. The leakage air streams at the kiln interfaces represent the greatest proportion within that category (50 %) hence improving the sealing between C1 and kiln as well as between kiln and PH zone will result in a considerable efficiency gain. Recapitulating, the gases that are heated by the process consist of three shares. Among these, the leakage air represents the category that needs to be reduced in order to increase the process efficiency.

The total heat in the hot off gases (~55 MW) composes of the heat contained in each of the four main gas streams as they leave the grate. Since the gas streams two to four, contribute 25 % to the total waste heat, gas stream one which leaves the PH zone represents the dominating part. In addition to that it should be pointed out that the temperature of the latter is around 450 °C and hence the contained heat is more valuable compared with the heat contained in the gas streams two to four. Summing up, in order to make better use of the hot off gases, the utilization of the heat contained in gas stream one represents the most effective measure to deal with.

## 5.2 Grate

Figure 5-3 shows the material flows as well as the occurring phenomena for the first process part. During the grate, the green pellets are completely dried and the calcium carbonate conversion is almost finished. The pellets leave the grate with an average fractional oxidation of around 60 %.



**Figure 5-3** Thermodynamic overview about the grate

Summarising the heat flows and the chemical reactions, the heat sources and heat sinks are calculated and presented in Figure 5-4. On the grate, hot air and flue gases dominate the heat supply (75 %), whereas the warming up of the pellets consumes most of the heat (75 %). In total there are 167 MW transferred.

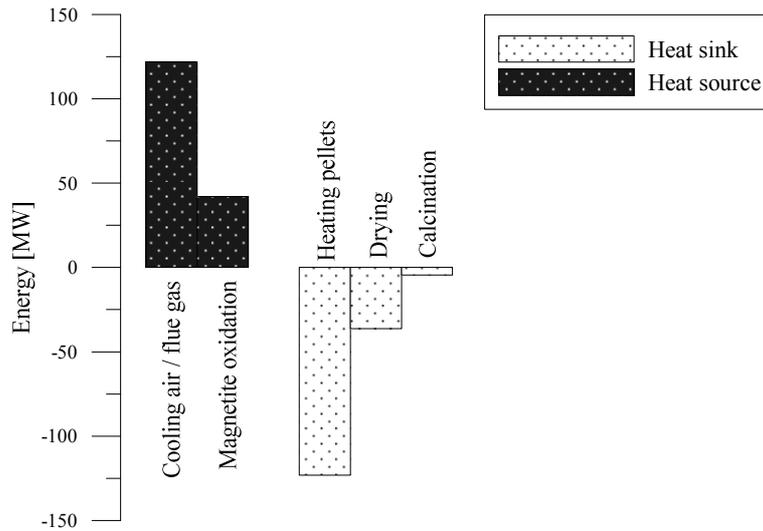


Figure 5-4 Heat sources and heat sinks of the grate

### 5.3 Kiln

Inside the kiln, coal is combusted for a further increase of the pellet temperatures in order to sinter the pellets. Due to the fact, that the influence of the sintering is not considered in the model, it is not included in the performed assessment and hence not in Figure 5-5. Taking into account the heat release from the magnetite oxidation and the considered radiative heat losses, the heat sources and heat sinks are drawn in Figure 5-6.

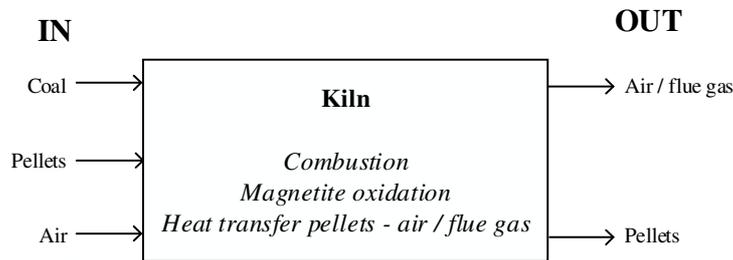


Figure 5-5 Thermodynamic overview about the kiln

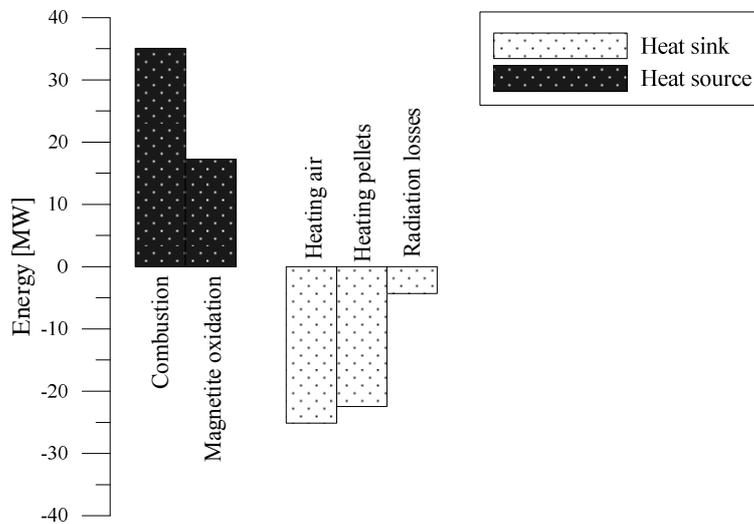
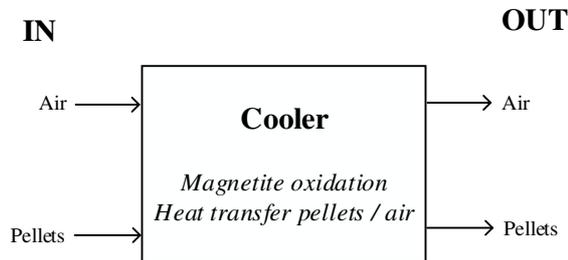


Figure 5-6 Heat sources and heat sinks of the kiln

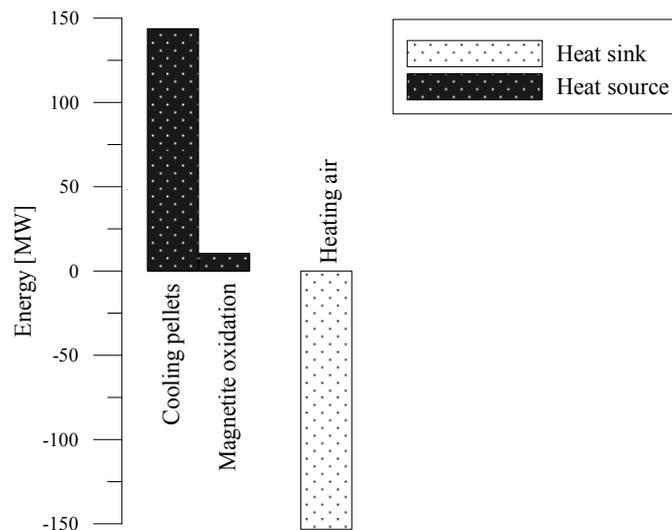
## 5.4 Cooler

During their progress within the cooler, the pellets are cooled down to nearly ambient temperature and an additional amount of magnetite is oxidized to hematite. A thermodynamic overview is provided in Figure 5-7.



**Figure 5-7** Thermodynamic overview about the cooler

Considering the two main material streams as well as the magnetite oxidation, the heat source and heat sinks diagram could be drawn as presented in Figure 5-8. In total there are around 155 MW transferred between the hot pellets out of the kiln and the cold ambient air. The heat release by the magnetite oxidation contributes only 7 % to the heat sources. Therefore the cooler thermodynamic characteristic could be simplified to heat exchange between hot pellets and cold ambient air.



**Figure 5-8** Heat sources and heat sinks of the cooler

## 6 Conclusion

This work aimed at developing a thermodynamic model of the Grate-Kiln process for the thermal treatment of iron ore pellets. This model is based on a Grate-Kiln unit at the LKAB mine site in Kiruna. Due to the large scope and complexity of the process, the relation between the predictability, usability and the level of detail is crucial to the model.

The possibilities for modelling chemical reactions are limited in the software EBSILON professional 10.0 used. For this reason, several subroutines were implemented by the usage of programmable components. The developed model is able to deal with the temperature differences within the pellet bed on the grate as well as on the cooler. In addition to that, the opportunity to investigate changes in the main magnetite oxidation influencing parameters is given.

The model is used to estimate the quantity of a series of process parameters that are not directly measurable. This category consists mainly of air streams that are drawn into the process and mixing air streams between bordering process sections. The result show that the leakage air streams at the kiln interfaces represent 50 % of the total amount of air that is drawn into the process. Furthermore, 20 % of the total flue gas entering the PH zone streams into the THP zone, most probably due to the fact that the flue gas out of the kiln is blown into the PH zone horizontally instead of vertically as in the case of the other grate zones.

The thermodynamic assessment of the process delivers a detailed analysis about the mass and heat transfer between the process parts. For each of the parts as well as for the whole process, all considered heat sinks and heat sources are presented. It was shown that the magnetite oxidation dominates the total heat supply with a share of around 66 %. Furthermore, the thermodynamic assessment reveals that either sealing enhancements at the kiln interfaces in order to reduce the leakage air at these positions, or utilization of the hot off gases that leaves the PH zone provides the greatest potential for process efficiency improvements.



## 7 Future work

This thesis presents the development of a thermodynamic model of the Grate-Kiln process. Due to the complex process, several simplifications were implemented. The validation proves the model's ability to reproduce qualitative results. In order to shift the model's usability more towards quantitative applications, the accuracy needs to be improved. Possible ways for enhancing the precision of the model are presented below.

Within the process, the magnetite oxidation represents the main phenomenon. The rate of the magnetite oxidation determines the amount of heat released. Due to the fact that two thirds of the total heat is supplied by this oxidation, the behaviour of the process is strongly influenced by the oxidation. The implemented oxidation function needs to be enhanced and adapted to take into account additional boundary conditions like the composition or the properties of the pellets.

The modelling of the chemical interactions within the process represents another field for improvements. By implementing all material flows with its actual contained species, instead of the currently applied definition by the constant specific heat, the ongoing chemical reactions as well as the thermodynamic behaviour of the materials could be described more thoroughly.

Finally, besides the already provided overall assessment of the process, one should focus on the modelling of one of the three process parts. The pellet bed on the grate for instance needs to be modelled and evaluated more particular. In this case, the current generic model could be used for providing the boundary conditions for the more detailed one. Otherwise the outcome of the more detailed model represents data for the adaptation of the generic one. Hence, both modelling approaches will benefit from each other and could be used simultaneously.



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## APPENDIX A - Subroutines used in the macros

Inside each macro, several subroutines are implemented via Kernel Scripting component (Component 93). The following chapters explain the three subroutines that are used in the model. Further on, the complete code for each subroutine is provided.

At the beginning of each modelling run, the total heat which is released during complete oxidation ( $\dot{Q}_{ox,total}$ ) needs to be calculated and fed to the model. The determined heat as calculated in equation A-1 is depending on the magnetite content in the green pellets ( $x_{mag}$ ), the total green pellet mass flow ( $\dot{m}_p$ ), the magnetite oxidation reaction heat ( $\Delta H_{ox}$ ) and the molar mass of magnetite ( $M_{mag}$ ).

$$\dot{Q}_{ox,total} = \frac{\dot{m}_p * x_{mag} * \Delta H_{ox}}{M_{mag}} \quad A-1$$

Similar to the oxidation of the magnetite, the total heat which is consumed by complete calcination of the calcium carbonate ( $\dot{Q}_{calc,total}$ ) must be determined and incorporated into the model. According to equation A-2, the calcium carbonate content in the green pellets ( $x_{CaCO_3}$ ), the total green pellet mass flow ( $\dot{m}_p$ ), the calcination reaction heat ( $\Delta H_{calc}$ ) and the molar mass of calcium carbonate ( $M_{CaCO_3}$ ) are used for this calculation.

$$\dot{Q}_{calc,total} = \frac{\dot{m}_p * x_{CaCO_3} * \Delta H_{calc}}{M_{CaCO_3}} \quad A-2$$

### Pellet drying

The modelled influence of the green pellet moisture evaporation during their progress on the grate is twofold. First, heat is reduced from the gas stream. Second the water that evaporates is reduced from the water stream. The mass transfer of water within the pellet bed on the grate caused by the evaporation and the condensation within the different grate layers is neglected. The implemented subroutine is based on the main simplification that the temperature of the water is kept constant, with independence of the pellet temperature. In addition, the parameters of the outgoing steam are considered to be continuous 100 °C and 1 bar.

When the subroutine is called, the temperature difference ( $\Delta T$ ) between the pellets and the air flow is calculated as follows.

$$\Delta T = T_p - T_{air} \quad A-3$$

Afterwards, the heat flow that is “available” for evaporation ( $\dot{Q}_{eva}$ ) is determined.

$$\dot{Q}_{eva} = \Delta T * c_{p,air} * \dot{m}_{air} \quad A-4$$

Right now, the outgoing water mass flow ( $\dot{m}_{water,out}$ ) reduced by the mass flow of evaporating water ( $\dot{m}_{water,eva}$ ) could be intended.

$$\dot{m}_{water,out} = \dot{m}_{water,in} - \frac{\dot{Q}_{eva}}{c_{p,water} * (100 - T_{water}) + h_{eva}} \quad A-5$$

Finally, the enthalpy of the outgoing air stream needs to be lowered by the enthalpy that was used for evaporation.

$$h_{air,out} = h_{air,current} - \frac{\dot{Q}_{eva}}{\dot{m}_{air}} \quad A-6$$

Table A-1 lists all the depending parameter that are read in by the drying subroutine as well as the parameters that are changed and given out.

**Table A-1** Parameters that are read in and changed by the drying subroutine

Medium	read parameter	set parameter
Air	$\dot{m}_{air,in}$	-
	$T_{air}$	-
	$h_{air,current}$	$h_{air,new}$
Pellet	$T_p$	-
Water	$\dot{m}_{water,current}$	$\dot{m}_{water,new}$

### Magnetite oxidation

The magnetite oxidation subroutine is the most complex and simultaneously the most crucial one. The reaction kinetics is based on the approximated oxidation curves provided in Chapter 4.2.

The subroutine starts with the conversion of the oxygen mass fraction in the gas flow ( $x_{O_2}$ ) to a volume concentration ( $C_{O_2}$ ). Equation A-7 is used for this purpose.

$$C_{O_2} = \frac{x_{O_2} * M_{air}}{M_{O_2}} \quad A-7$$

Right now, the oxidation oxygen factors a, b and c needs to be calculated according to equations A-8 to A-10.

$$a = 10^{-5} * C_{CO}^2 - 4 * 10^{-6} * C_{O_2} - 2 * 10^{-8} \quad A-8$$

$$b = 0.133 * C_{O_2}^3 - 0.008 * C_{CO}^2 + 0.017 * C_{O_2} - 0.0002 \quad A-9$$

$$c = -36.93 * C_{O_2}^3 + 20.38 * C_{CO}^2 - 4.32 * C_{O_2} + 0.0423 \quad A-10$$

Within the kiln, the duration time of the pellets differs from the time where the pellets are directly exposed to the oxygen carrying gas. To take this circumstance into account, a limiting factor (lim) according to equation A-11 is introduced. For the kiln, this factor is set to 0.75, whereas an unlimited expose time for the grate and for the cooler is assumed (lim = 1).

$$t_s = t * lim \quad A-11$$

In order to determine the new fractional oxidation of the pellets ( $F_{ox,new}$ ) with formula A-12, the current fractional oxidation ( $F_{ox,current}$ ) is transferred to an additional time ( $t_{ox}$ ) as defined in equation A-13.

$$F_{ox,new} = (t_s + t_{ox})^{0.25} * (a * T_p^2 + b * T_p + c) \quad A-12$$

$$t_{ox} = \left( \frac{F_{ox,current}}{a * T_p^2 + b * T_p + c} \right)^4 \quad A-13$$

The reaction heat that is released by the oxidation ( $\dot{Q}_{ox}$ ) in the component is determined by equation A-14. Depending on the considered layer, the corresponding layer factor (l) is either 0.2 for the bottom and top layer or 0.6 for the middle layer on the grate. Within the cooler, the used layer factors are 0.066 for the top and bottom layer and 0.868 for the middle layer. The two different sets of layer factors are caused by the change in the layer distribution of mass flows and oxidation levels between kiln and cooler (Chapter 4.3).

$$\dot{Q}_{ox} = (F_{ox,new} - F_{ox,current}) * \dot{Q}_{ox,total} * l \quad A-14$$

The new enthalpy of the outgoing pellets flow ( $h_{p,new}$ ) results from equation A-15.

$$h_{p,new} = \frac{\dot{Q}_{ox}}{\dot{m}_p} + h_{p,current} \quad \text{A-15}$$

To reduce the oxygen mass fraction within the air flow, the mole flow of the oxidizing magnetite ( $\dot{n}_{mag}$ ) needs to be determined.

$$\dot{n}_{mag} = \frac{(F_{ox,new} - F_{ox,current}) * \frac{1}{M_{mag}}}{\dot{m}_p} \quad \text{A-16}$$

According to the chemical reaction provided in Chapter 4.2 the mass flow of oxygen that is bounded in the pellets is calculated and removed from the current air mass flow to set the new air mass flow ( $\dot{m}_{air,new}$ ).

$$\dot{m}_{air,new} = \dot{m}_{air,current} - \frac{\dot{n}_{mag}}{4} * M_{O_2} \quad \text{A-17}$$

In order to define the new composition of the involved air flow, the four main air components are considered namely, nitrogen, oxygen, carbon dioxide and argon. For all listed components the new mass fractions ( $x_{i,new}$ ) needs to be specified.

$$x_{i,new} = \frac{x_{i,current} * \dot{m}_{air,current}}{\dot{m}_{air,new}} \quad \text{A-18}$$

Finally, as well as in the previous chapter, Table A-2 provides all depending parameters that are read in, as well as the parameters that are changed during the subroutine and given out in the end.

**Table A-2** Parameters that are read in and changed by the magnetite oxidation subroutine

Medium	read parameter	set parameter
Air	$x_{O_2,current}$	$x_{O_2,new}$
	$x_{N_2,current}$	$x_{N_2,new}$
	$x_{CO_2,current}$	$x_{CO_2,new}$
	$x_{Ar,current}$	$x_{Ar,new}$
Flue gas	$\dot{m}_{air,current}$	$\dot{m}_{air,new}$
Pellet	$T_p$	-
	$\dot{m}_{p,current}$	-
	$F_{Ox,current}$	$F_{Ox,new}$
	$h_{p,current}$	$h_{p,new}$
-	$t_s$	-
-	$\dot{Q}_{Ox,total}$	-

### Calcination of calcium carbonate

The approach of the calcination subroutine is similar to the oxidation ones. The basic assumptions behind the implemented kinetics are described in Chapter 4.2.

In order to calculate the consumed reaction heat, the new calcination level ( $F_{calc,new}$ ) must be determined. If the pellet temperature exceeds 600 °C the new calcination level could be calculated according to equation A-19.

$$F_{calc,new} = \sqrt{T_p - 600} * 6 \quad \text{A-19}$$

Right now, the consumed heat ( $\dot{Q}_{calc}$ ) is specified as shown in equation A-20. Depending on the considered layer, the corresponding layer factor is either 0.2 or 0.6.

$$\dot{Q}_{calc} = \frac{(F_{calc,new} - F_{calc,current})}{100} * \dot{Q}_{calc,total} * l \quad A-20$$

The new enthalpy of the outgoing pellets flow ( $h_{p,new}$ ) is determined according to equation A-21.

$$h_{p,new} = \frac{\dot{Q}_{calc}}{\dot{m}_p} + h_{p,current} \quad A-21$$

All model depending parameter that were either used or changed during the calcination subroutine are summarised in **Table A-3**.

**Table A-3** Parameters that are read in and changed by the calcination subroutine

Medium	read parameter	set parameter
	$T_p$	-
Pellets	$h_{p,current}$	$h_{p,new}$
	$\dot{m}_{p,in}$	-
	$F_{calc,current}$	$F_{calc,new}$
-	$\dot{Q}_{calc,total}$	-

### Combined calcination and magnetite oxidation

During the grate and the kiln, the heat release of the oxidation as well as the heat consumed by the calcination needs to be considered. To do so, both subroutines are running simultaneously, hence the new pellets enthalpy comprises both reaction heats as shown by equation (A-22).

$$h_{p,new} = h_{p,current} + \frac{\dot{Q}_{ox} + \dot{Q}_{calc}}{\dot{m}_p} \quad A-22$$

### Subroutine codes

This section presents the program codes that are used in the Kernel Scripting components. The associated explanations are written in italic.

#### Drying subroutine

```

uses @kernelscripting, @fluid;                                     //interface definition
var                                                                //variable definition(real)
pair1, mair1, hair1, qneed, waterleft, tair1, tpellets, twater, evaE, totalevaE, cpair, cpwater, deltat, qfree,
mwater1, pwater1, hwater1, hfree, hnew,O2,CO2,Ar,N2:real;
FData:FluidData;                                                //variable definition (FluidData)
begin                                                            //start drying subroutine
evaE := 2260;                                                    // evaporation enthalpy water [kJ/kg]
cpair := 1.005;                                                 // cp air [kJ/kg*K]
cpwater := 4.186;                                              // cp water [kJ/kg*K]
ksGetInPipeFluidData(1, FData);                                  //read in air composition
O2:= FData.fluidAnalysis[SubstanceO2];                          //mass fraction oxygen
N2:= FData.fluidAnalysis [SubstanceN2];                         //mass fraction nitrogen
CO2:= FData.fluidAnalysis[SubstanceCO2];                       //mass fraction carbon dioxide
Ar:= FData.fluidAnalysis[SubstanceAr];                          //mass fraction argon
tpellets:= PIn.T;                                               //read in pellets temperature [°C]
tair1 := AirIn.T;                                               //read in air temperature [°C]
twater := water.T;                                              //read in water temperature [°C]
hair1 := ksGetInPipeValue (1, PhysValueH);                     //read in pellets enthalpy [kJ/kg]
mair1 := ksGetInPipeValue (1, PhysValueM);                     //read in pellets mass flow [kg/s]
pair1 := ksGetInPipeValue (1, PhysValueP);                     //read in pellets pressure [bar]
mwater1 := ksGetInPipeValue (2, PhysValueM);                   //read in water mass flow [kg/s]

```

```

pwater1 := ksGetInPipeValue (2, PhysValueP);           //read in water pressure [bar]
hwater1 := ksGetInPipeValue (2, PhysValueH);           //read in water enthalpy [kJ/kg]
evaE := evaE + (100-twater)*cpwater;                 //enthalpy (heating/evaporating water) [kJ/kg]
totalevaE := mwater1 * evaE;                          //needed heat (evaporating / heating) [kW]
tpellets:= tpellets +1;                               //buffer degree
ksSetOutPipeValue (1, PhysvalueM, mair1);             //set out air mass flow (constant) [kg/s]
ksSetOutPipeValue (1, PhysvalueP, pair1);             //set out air pressure (constant) [bar]
ksSetOutPipeValue (2, PhysvalueH, hwater1);          //set out water enthalpy (constant) [kJ/kg]
ksSetOutPipeValue (2, PhysvalueP, pwater1);          //set out water pressure (constant) [bar]
if (mair1 >0) then                                     //air must be warmer then pellets
  begin
    if (tair1 > 100)                                   //air must be warmer than 100 °C
    then
      begin
        deltat := tair1 - tpellets;                   //”available” temperature dif. [°C]
        if (deltat > 0)then                             //temperature dif. must be positive
        begin
          qfree:=deltat*cpair*mair1;                   //available heat for evaporation [kW]
          if (qfree > totalevaE) then                   //available heat > needed heat
          begin
            hfree := totalevaE / mair1;                //used enthalpy for evap. [kJ/kg]
            hnew := hair1 - hfree;                     //new air enthalpy [kJ/kg]
            ksSetOutPipeValue (1, PhysvalueH, hnew);
            //set out new air enthalpy [kJ/kg]
            ksSetOutPipeValue (2, PhysvalueM, 0);
            //set out water mass flow (0) [kg/s]
          end
          else
            //available heat < needed heat
          begin
            hfree := qfree / mair1;                    //used enthalpy for evap. [kJ/kg]
            hnew := hair1 - hfree;                     //new air enthalpy [kJ/kg]
            waterleft := mwater1 - (qfree / totalevaE) * mwater1;
            //new water mass flow [kg/s]
            ksSetOutPipeValue (1, PhysvalueH, hnew);
            //set out air enthalpy [kJ/kg]
            ksSetOutPipeValue (2, PhysvalueM, waterleft);
            // set out water mass flow [kg/s]
          end;
        end
        else
          //temperature dif. negative
          begin
            //no evaporation
            ksSetOutPipeValue (1, PhysvalueH, hair1);  //set out air enthalpy [kJ/kg]
            ksSetOutPipeValue (2, PhysvalueM, mwater1); //set out water mass flow [kg/s]
          end;
        end
        else
          //air colder than 100 °C
          begin
            //no evaporation
            ksSetOutPipeValue (1, PhysvalueH, hair1);  //set out air enthalpy [kJ/kg]
            ksSetOutPipeValue (2, PhysvalueM, mwater1); //set out water mass flow [kg/s]
          end;
        end
        else
          //air colder than pellets
          begin
            //no evaporation
            ksSetOutPipeValue (1, PhysvalueH, hair1);  //set out air enthalpy [kJ/kg]
            ksSetOutPipeValue (2, PhysvalueM, mwater1); //set out water mass flow [kg/s]
          end;
        end
      end
    end
  end
  ksSetOutPipeFluidData (1,Fdata);                    //set out air composition (constant)
end.                                                    //end drying subroutine

```

## Combined calcination oxidation component

```

uses @kernelscripting, @fluid; //interface definition
var //variable definition (real)
temp, degree, time, oxE, OxEt, OxELay, mp, hp, pp, O2, N2, CO2, Ar, vo2, mO2, mN2, mCO2,
mAr, mair, hair, pair, a, b, c, t1, degree1, deltadegree, deltah, O2loss, MMag, MolO2, OxM, OxR,
deltacalc, calcdegree, calc, calcEt, calcELay, calcE, lim :real;
FData: FluidData; //variable definition (FluidData)
begin //start calcination / oxidation subroutine
mp :=ksGetInPipevalue (2,PhysvalueM); //read in pellets mass flow [kg/s]
hp :=KsGetInPipevalue (2,PhysvalueH); //read in pellets enthalpy [kJ/kg]
pp :=ksGetInPipevalue (2,PhysvalueP); //read in pellets pressure [bar]
degree := ksGetInPipevalue (3, PhysvalueM); //read in oxidation degree [%]
calcdegree := ksGetInPipevalue (3, PhysvalueP); //read in calcination degree [%]
time:= ksGetInPipevalue (4, PhysvalueM); //read in section time [min]
OxEt := ksGetInPipevalue (6, PhysvalueM); //read in total oxidation heat [MW]
calcEt := ksGetInPipevalue (5, PhysvalueM); //read in total calcination heat [MW]
temp:= POx.T; //read in pellets temperature [°C]
mair := ksGetInPipevalue (1, PhysvalueM); //read in air mass flow [kg/s]
hair := ksGetInPipevalue (1, PhysvalueH); //read in air enthalpy [kJ/kg]
pair := ksGetInPipevalue (1, PhysvalueP); //read in air pressure [bar]
ksGetinPipeFluidData (1, FData); //read in air composition
O2 := FData.fluidAnalysis[SubstanceO2]; //oxygen mass fraction
N2 := FData.fluidAnalysis[SubstanceN2]; //nitrogen mass fraction
CO2 := FData.fluidAnalysis[SubstanceCO2]; //carbon dioxide mass fraction
Ar := FData.fluidAnalysis[SubstanceAr]; //argon mass fraction
MMag := 231.539; //define molar mass magnetite [g/mol]
MOIO2 := 31.999; //define molar mass oxygen [g/mol]
Lim := 0.75; //define limiting factor for the kiln [-]
calcElay := calcEt * 1000*0.2; //scaling calc. heat bottom layer [kW]
OxElay := OxEt * 1000 * 0.2; //scaling oxidation heat bottom layer [kW]
mO2 := O2 * mair; //calculation mass flow oxygen [kg/s]
degree := degree/100; //scaling oxidation degree [%/100]
time := time * lim; //calculation of the actual expose time [min]
vo2:=(o2*28.96)/31.99; //calculation oxygen concentration
if (temp>300) then //magnetite oxidation starts at 300 °C
begin
a := 0.00001*vO2*vO2 - 0.000004*vO2 - 0.00000002; //oxidation factor a [-]
b := 0.1333*vO2*vO2*vO2-0.08*vO2*vO2+0.0177*vO2-0.0002; //oxidation factor b[-]
c := -36.933*vO2*vO2*vO2+20.38*vO2*vO2-4.3267*vO2+0.0423; //oxidation factor c [-]
t1 := pow(degree/((a*temp*temp)+(b*temp)+c),4); //additional time [min]
degree1:= pow((t1+time),0.25)*((a*temp*temp) + b*temp + c); //new oxidation degree
if (degree1 < 1) then
begin
deltadegree := degree1-degree; //deltadegree if new oxidation degree <1
end
else
begin
deltadegree := 1-degree; //deltadegree if new oxidation degree >1
degree1 := 1; //setting new oxidation degree to 1
end;
end
else //no magnetite oxidation
begin
deltadegree := 0; //deltadegree if temp < 300 °C
degree1 := degree; //new oxidation degree = old oxidation degree
end;
OxE := deltadegree * OxElay; //released oxidation heat [kW]
mN2 := N2 * mair; //mass flow nitrogen [kg/s]
mCO2 := CO2 * mair; //mass flow carbon dioxide [kg/s]
mAr := mair - mN2 - mO2 - mCO2; // mass flow argon [kg/s]

```

```

OxM := deltadegree * mp; //reacting magnetite mass flow [kg/s]
OxM := OxM / MMag; //reacting magnetite molar flow [mol/s]
OxR := OxM / 4; //reacting oxygen molar flow [mol/s]
OxR := OxR * molO2; //reacting oxygen mass flow [kg/s]
mO2 := mO2 - OxR; //new oxygen mass flow [kg/s]
mair := mair - OxR; //new air mass flow [kg/s]
O2 := mO2 / mair; //new oxygen mass fraction
N2 := mN2 / mair; //new nitrogen mass fraction
CO2 := mCO2 / mair; //new CO2 mass fraction
Ar := 1 - CO2 - N2 - O2; //new argon mass fraction
if (temp > 600) then //calcination starts at 600 °C
begin
calc := pow((temp-600),0.5)*6; //new calcination degree
if (calc <100) then
begin
deltacalc := calc - calcdegree; //deltacalc if new calc. degree <100 %
end
else
begin
deltacalc := 100 - calcdegree; //deltacalc if new calc. degree >100 %
calc := 100; //setting new calcination degree to 100 %
end;
end
else
begin
deltacalc := 0; //deltacalc if temp below 600 °C
calc := 0; //calcination degree below 600 °C
end;
calcE := (deltacalc/100) * calcElay; //consumed calcination heat [kW]
calcdegree := calc; //setting new calcination degree
deltah := (OxE - CalcE) / mp; //resulting heat oxidation +calcination [kJ/kg]
hp := hp + deltah; //new pellets enthalpy
kssetoutpipevalue(2,PhysvalueM,mp); //set out pellets mass flow (constant) [kg/s]
kssetoutpipevalue(2,PhysvalueH,hp); //set out pellets enthalpy [kJ/kg]
kssetoutpipevalue(2,PhysvalueP,pp); //set out pellets pressure (constant) [bar]
kssetoutpipevalue(5,PhysvalueM,degree1*100); //set out new oxidation degree [%]
kssetoutpipevalue(5,PhysvalueP,calcdegree); //set out new calcination degree [%]
kssetoutpipevalue (1,PhysvalueM,mair); //set out air mass flow [kg/s]
kssetoutpipevalue (1,PhysvalueP,pair); //set out air pressure (constant) [bar]
kssetoutpipevalue (1,PhysvalueH,hair); //set out air enthalpy (constant) [bar]
FData.fluidAnalysis[SubstanceO2]:=O2; //set oxygen mass fraction
FData.fluidAnalysis[SubstanceCO2]:=CO2; //set carbon dioxide mass fraction
FData.fluidAnalysis[SubstanceAr]:=Ar; //set argon mass fraction
FData.fluidAnalysis[SubstanceN2]:=N2; //set nitrogen mass fraction
kssetoutpipeFluidData (1, Fdata); //set out air composition
end. //end oxidation / calcination subroutine

```



# APPENDIX B - Grate-Kiln model overview

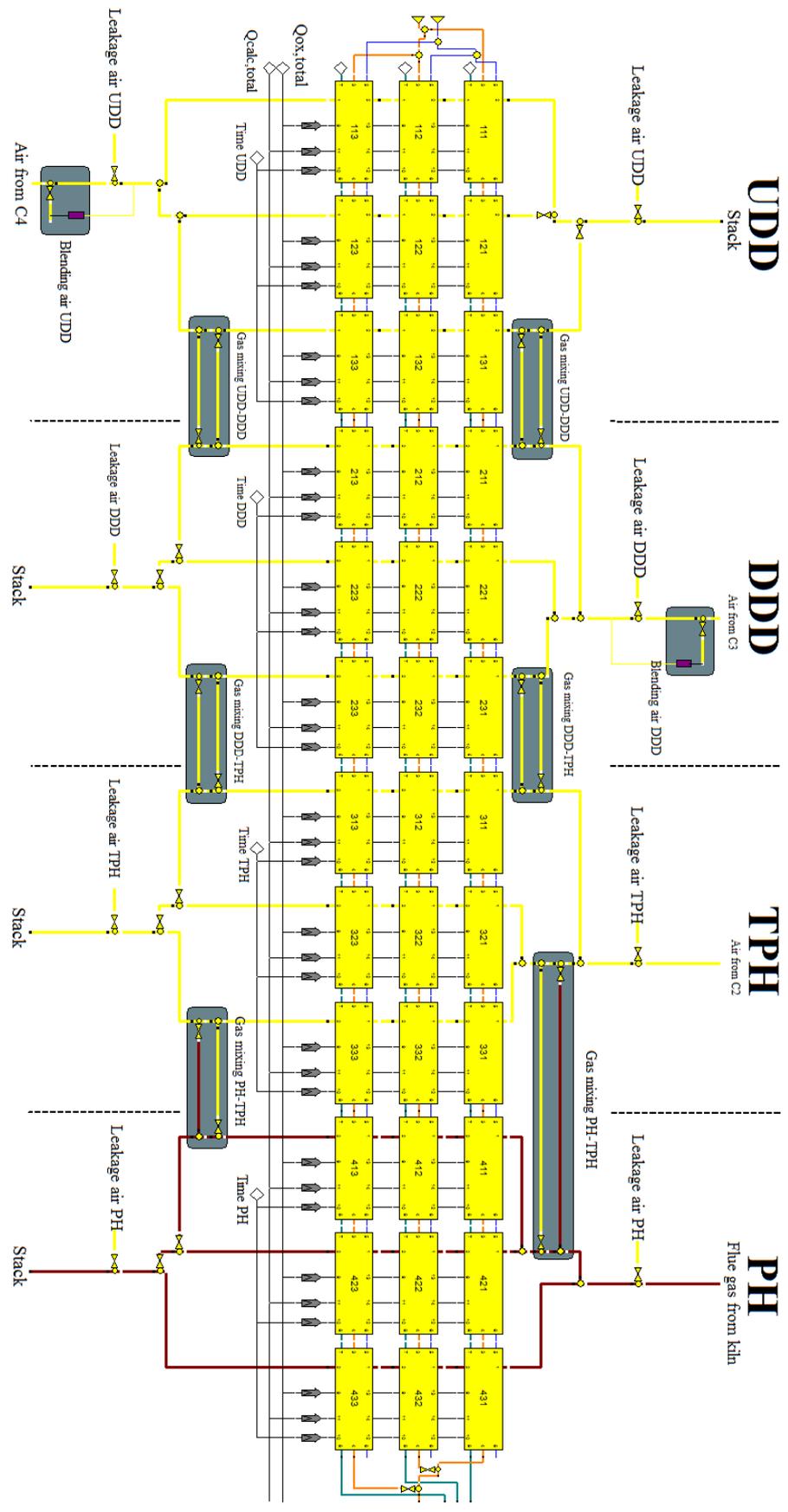
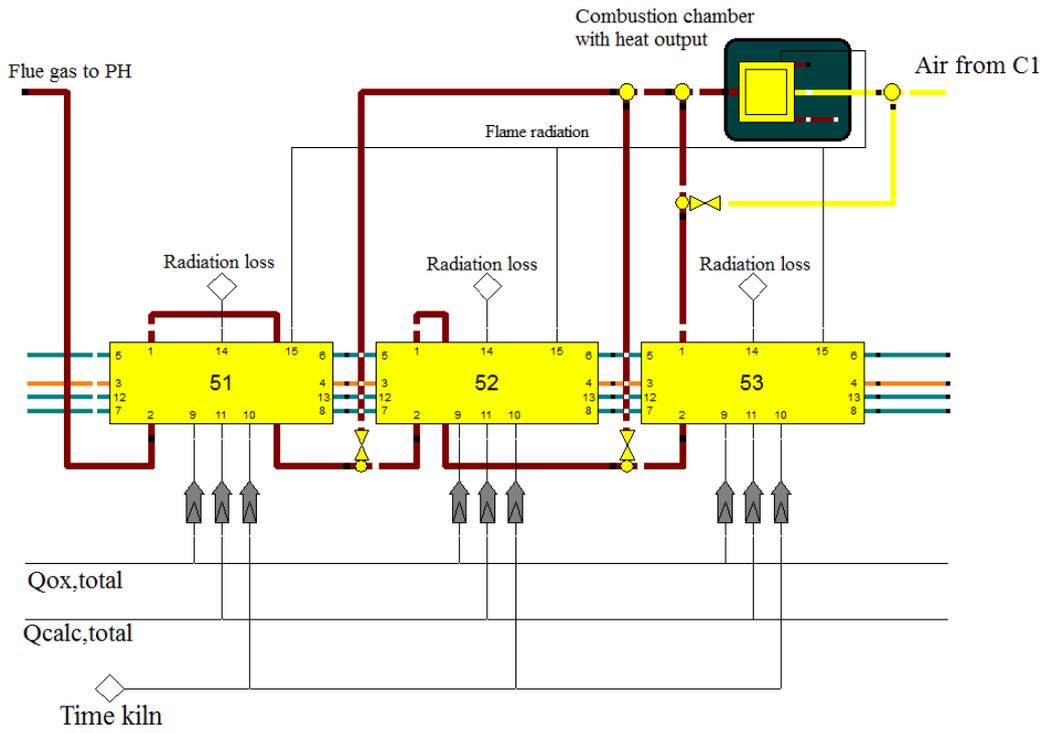


Figure B-1 Illustration of the Grate-Kiln model (grate)



**Figure B-2** Illustration of the Grate-Kiln model (kiln)

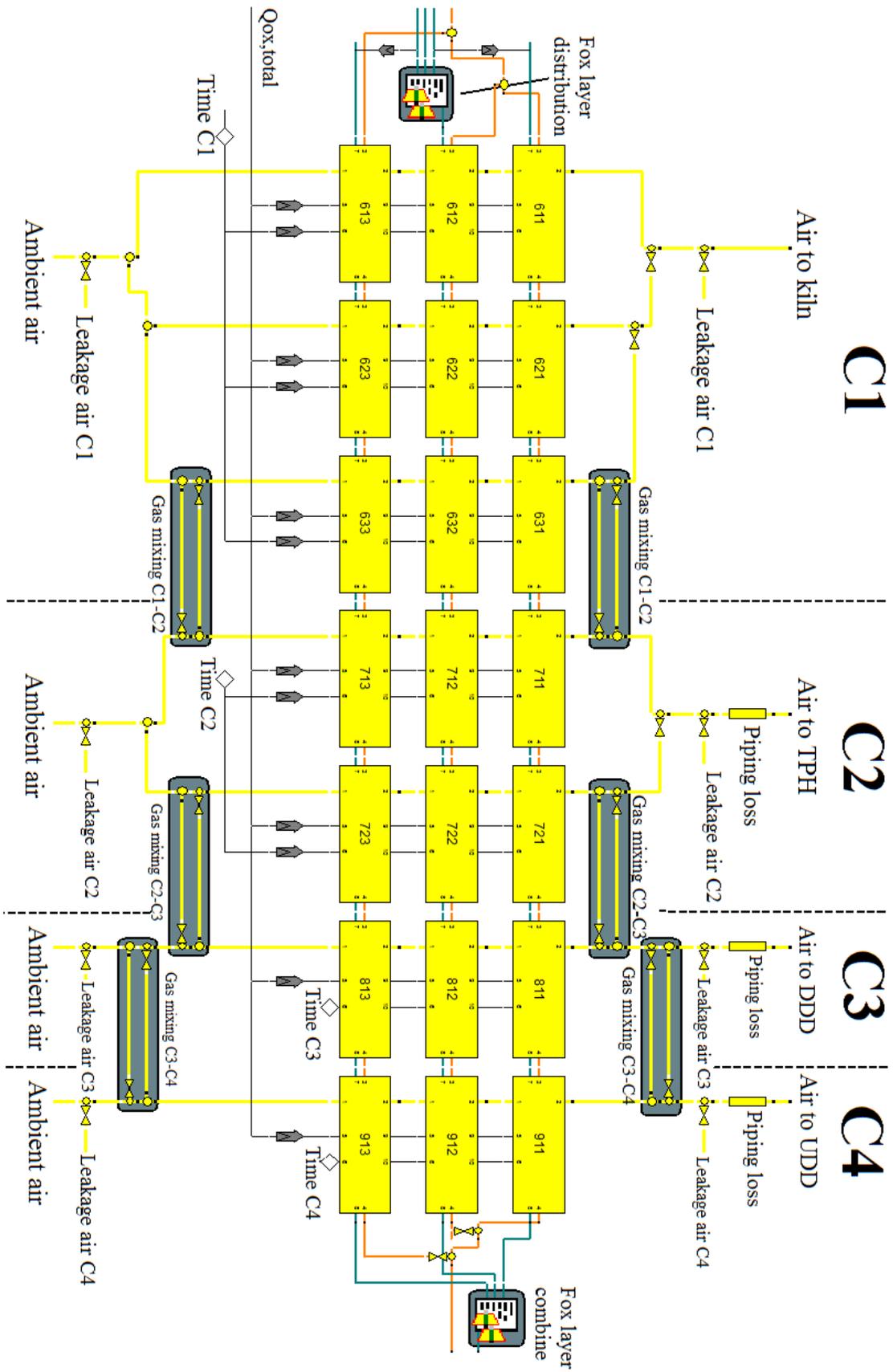
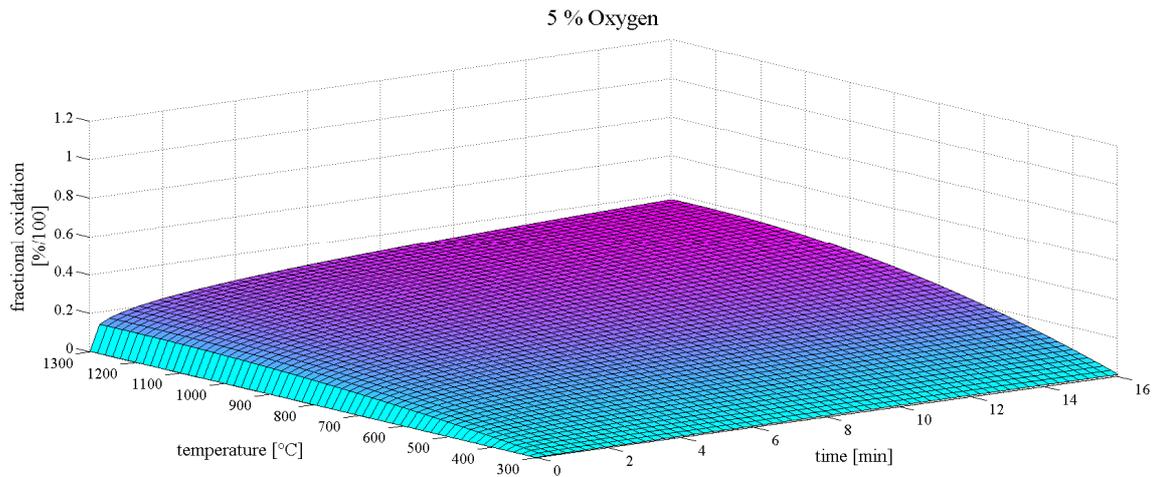


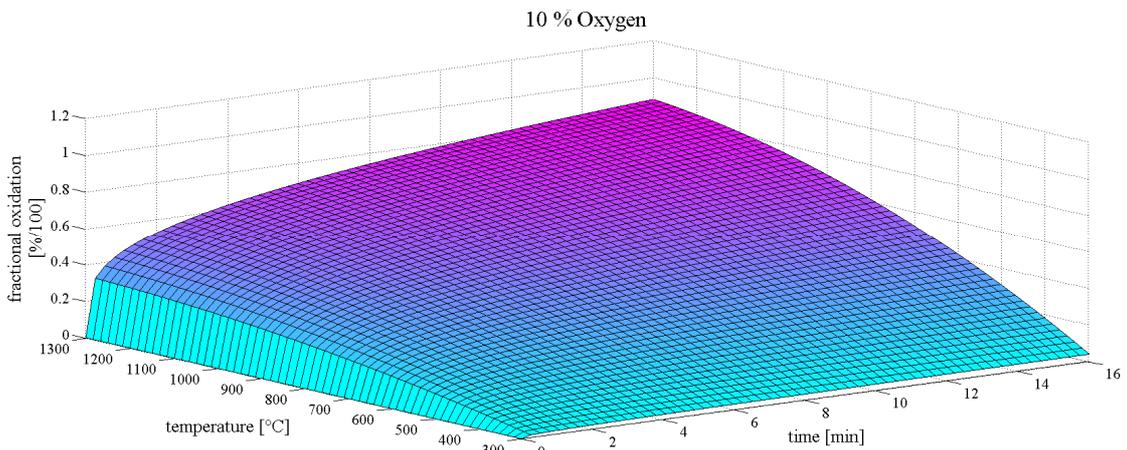
Figure B-3 Illustration of the Grate-Kiln model (cooler)



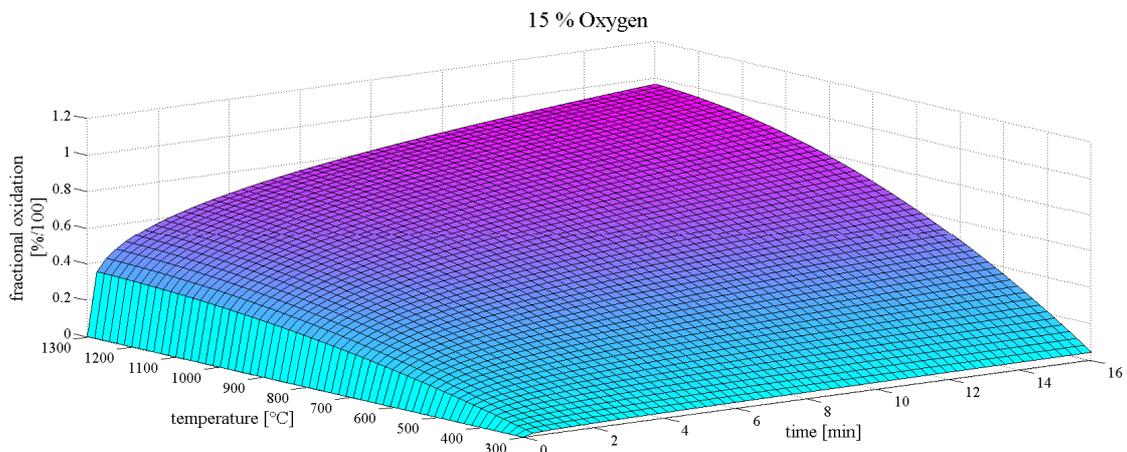
## APPENDIX C - Magnetite oxidation curves



**Figure C-1** Fractional magnetite oxidation depending on pellet temperature and roasting time for 5 % oxygen in the surrounding gas



**Figure C-2** Fractional magnetite oxidation depending on pellet temperature and roasting time for 10 % oxygen in the surrounding gas



**Figure C-3** Fractional magnetite oxidation depending on pellet temperature and roasting time for 15 % oxygen in the surrounding gas



## Appendix D - Tables referring to Chapter 5

In addition to the figures already presented in Chapter 5, this appendix provides tables, that include all the considered mass and heat flows as well as tables with the heat sinks and heat sources within the entire Grate-Kiln process and its process parts.

**Table D-1** Heat and material flows Grate-Kiln process

Stream	$\dot{m}_{in}$ [kg/s]	$T_{in}$ [°C]	$\dot{Q}_{in}$ [MW]	$\dot{m}_{out}$ [kg/s]	$T_{out}$ [°C]	$\dot{Q}_{out}$ [MW]
Air stream 1	55.0	0.0	0.0	79.4	472.5	43.2
Air stream 2	45.0	0.0	0.0	54.8	67.0	3.8
Air stream 3	40.0	0.0	0.0	49.4	87.4	4.3
Air stream 4	125.0	0.0	0.0	216.9	24.5	5.3
Air <sub>leakage</sub>	53.0	25.0	1.3	-	-	-
Air <sub>blending</sub>	85.3	0.0	0.0	-	-	-
Steam	-	-	-	13.5	100.0	36.1
Green pellets	150.0	13.0	2.3	-	-	-
Final pellets	-	-	-	136.5	30.0	3.6
Coal	1.0	0.0	35.0	-	-	-

**Table D-2** Heat sources and heat sinks Grate-Kiln process

Description	abs. value	Unit	rel. value	Unit
Heating air	55.4	MW	52.9	%
Heating pellets	2.0	MW	2.0	%
Drying	35.4	MW	33.8	%
Calcination	4.5	MW	4.3	%
Radiative heat losses	4.3	MW	4.1	%
Pipe losses	3.0	MW	2.9	%
<b>Σ Heat sinks</b>	<b>104.6</b>	<b>MW</b>	<b>100</b>	<b>%</b>
Magnetite oxidation	69.6	MW	66.5	%
Combustion	35.0	MW	33.5	%
<b>Σ Heat sources</b>	<b>104.6</b>	<b>MW</b>	<b>100</b>	<b>%</b>

**Table D-3** Heat and material flows grate

<b>Stream</b>	$\dot{m}_{in}$ [kg/s]	$T_{in}$ [°C]	$\dot{Q}_{in}$ [MW]	$\dot{m}_{out}$ [kg/s]	$T_{out}$ [°C]	$\dot{Q}_{out}$ [MW]
Air <sub>UDD</sub>	212.5	142.7	30.6	216.9	24.5	5.3
Air <sub>DDD</sub>	41.0	445.3	18.9	49.4	87.4	4.3
Air <sub>TPH</sub>	51.6	699.5	38.3	54.8	69.0	3.8
Flue gas <sub>PH</sub>	66.4	1190.7	88.1	79.4	472.5	41.2
Air <sub>Leakage</sub>	32.0	25	0.8	-	-	-
Green pellets	150.0	13	2.3	-	-	-
Pellets	-	-	-	136.5	1039.2	124.8
Steam	-	-	-	13.5	100	36.12

**Table D-4** Heat sources and heat sinks grate

<b>Description</b>	<b>abs. value</b>	<b>Unit</b>	<b>rel. value</b>	<b>Unit</b>
Heating pellets	123.3	MW	75.2	%
Drying	36.3	MW	22.1	%
Calcination	4.5	MW	2.7	%
<b>Σ Heat sinks</b>	<b>164.0</b>	<b>MW</b>	<b>100</b>	<b>%</b>
Magnetite oxidation	42.1	MW	25.7	%
Cooling air / flue gas	121.9	MW	74.3	%
<b>Σ Heat sources</b>	<b>164.0</b>	<b>MW</b>	<b>100</b>	<b>%</b>

**Table D-5** Heat and material flows kiln

Stream	$\dot{m}_{in}$ [kg/s]	$T_{in}$ [°C]	$\dot{Q}_{in}$ [MW]	$\dot{m}_{out}$ [kg/s]	$T_{out}$ [°C]	$\dot{Q}_{out}$ [MW]
Air / flue gas	66.5	875.7	63.0	66.4	1190.7	88.1
Pellets	136.5	1039.2	124.8	136.5	1226.1	147.3
Coal	1.0	0	35.0	-	-	-

**Table D-6** Heat sources and heat sinks kiln

Description	abs. value	Unit	rel. value	Unit
Heating air / flue gas	25.1	MW	48.5	%
Heating pellets	22.5	MW	43.3	%
Radiative heat losses	4.3	MW	8.2	%
<b><math>\Sigma</math> Heat sinks</b>	<b>51.9</b>	<b>MW</b>	<b>100</b>	<b>%</b>
Magnetite oxidation	16.9	MW	67.1	%
Combustion	35.0	MW	32.9	%
<b><math>\Sigma</math> Heat sources</b>	<b>51.9</b>	<b>MW</b>	<b>100</b>	<b>%</b>

**Table D-7** Heat and material flow cooler

<b>Stream</b>	$\dot{m}_{in}$ [kg/s]	$T_{in}$ [°C]	$\dot{Q}_{in}$ [MW]	$\dot{m}_{out}$ [kg/s]	$T_{out}$ [°C]	$\dot{Q}_{out}$ [MW]
Air <sub>C1</sub>	55.0	0	0	66.5	875.7	63.0
Air <sub>C2</sub>	45.0	0	0	51.6	717.1	39.3
Air <sub>C3</sub>	40.0	0	0	41.0	468.2	19.9
Air <sub>C4</sub>	125.0	0	0	127.2	245.2	31.7
Air <sub>Leakage</sub>	21.0	25.0	0.5	-	-	-
Pellets	136.5	1226.1	147.3	136.5	30.0	3.6

**Table D-8** Heat sources and heat sinks cooler

<b>Description</b>	<b>abs. value</b>	<b>Unit</b>	<b>rel. value</b>	<b>Unit</b>
Heating air	154.0	MW	100	%
<b>Σ Heat sink</b>	<b>154.0</b>	<b>MW</b>	<b>100</b>	<b>%</b>
Cooling pellets	143.7	MW	93.3	%
Magnetite oxidation	10.3	MW	6.7	%
<b>Σ Heat sources</b>	<b>154.0</b>	<b>MW</b>	<b>100</b>	<b>%</b>