Fingerprint of a submerged-arc Furnace

Optimising energy consumption through data mining, dynamic modelling and computational fluid dynamics

Proefschrift

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Die boek dra ek onvoorwaardelik op aan my geliefde familie
en my geliefde Eleonora
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Executive Summary

This study imparts a scientific perception of a phosphorous-producing submerged arc furnace never seen before; a proverbial fingerprint that can improve problem identification, disturbance diagnostics, process prediction, dynamic modelling and model predictive control of this type of furnace. It successfully incorporates accurate, multi-field thermodynamic-, kinetic- and industrial data with computational flow dynamic calculations; thus further unifying the sciences of kinetics and equilibrium thermodynamics. The true power of this study is the extensive and methodical validation that ensures industrially endorsed results. To facilitate all this the author spent six uninterrupted months at an industrial plant (Thermphos International), twice walked inside a cold submerged-arc furnace, gathered and analysed more than thirty-four mineralogical samples, managed an extensive and insightful sampling campaign on the slag streams, performed feed material porosity tests and had thirteen additional temperature probes installed inside the furnace lining. The author also scrutinised over years of industrial data, inspected many industrial drawing and partook in countless valuable conversations with industrial and technical experts to guarantee, not only a valuable scientific contribution, but one that is deep-rooted in authentic engineering principles.

The process The process under investigation is the large-scale production of phosphorus at Thermphos International. The main reaction is defined by the Wöhler process, producing a calcium-silicate slag, calcium fluoride, carbon monoxide and the desired product, phosphorus gas. Gravity delivers the feed, consisting of pelletised apatite, coke and silica (in the form of gravel), to a submerged arc furnace through ten, evenly distributed feed chutes ensuring a constant packed bed volume. The gaseous product leaves the furnace through two symmetrically spaced outlet vents situated above the ferrophosphorus tap hole in the roof of the furnace. The ferrophosphorus is tapped off, usually once per day. However, slag is continuously tapped through two alternating, water-cooled tapping holes located 400 mm above the furnace floor. Owing to the large production volume of slag, a seemingly small wt% of P₂O₅ in the slag (P₂O₅(slag)) results in substantial losses of unreduced, potential product.

Control Controlling the process in order to keep the P₂O₅(slag) as low as possible, is therefore one of the top priorities. For this reason P₂O₅(slag) was chosen as the predicted output variable in subsequent models. The furnace process is controlled automatically though a constant-current principle that utilises changing electrode
operating heights in order to stabilise the current. Apart from automated control, the ratio of fixed carbon-to-P$_2$O$_5$ (C-fix) addition, the ratio of silica gravel-to-pellets (silica gravel factor) addition and the ratio of coke-to-pellets (coke factor) addition are fully independent variables used as operator tools to steer and optimise the process. In order to quantitatively understand the influence of these and other more dependent variables, raw industrial data was investigated. A common practise in the phosphorous industry is to compensate for increased P$_2$O$_5$(slag) by increasing the C-fix in the packed bed, with the desired result a lower P$_2$O$_5$(slag) through additional reductive power available as a result of the additional coke. It was however proven that this action, contrary to the common perception, does not always have the desired effect. At constant Moeller flowrates, P$_2$O$_5$(slag) values were largely independent of C-fix and mostly a function of feed material residence time in the furnace.

**Data reconciliation and the optimum operating range** Owing to the fact that the slag-, ferrophosphorus- and P$_4$ flowrates are not directly measured, data reconciliation was performed around one of the furnaces over a six month period. In this way these flowrates were obtain in a real-time way and provided soft-sensor values. These values were then used in an operating cost analysis exercise revealing that the most profitable operating zone is at Moeller flowrates $\geq 25-30$ [ton/hour] AND C-fix $\leq 0.475$. Even though this was also the operating area with maximum P$_2$O$_5$(slag) losses, decreased electricity cost and not decreased P$_2$O$_5$(slag) remains the more dominant factor. This shows that the drive for lower SPC and not higher P$_4$ recovery provides larger profits.

**A Dynamic-CFD hybrid model** A phosphorus producing, submerged arc furnace is continuously fluctuating between the dynamic-driven state and the thermodynamic-driven. Therefore, one single modelling approach will never be sufficient and it becomes increasingly difficult for standard thermodynamic and kinetic modelling (as well as the associated software) to provide adequate support for any predictive dynamic model (Reuter and Yang, 2005). A combination of modelling techniques is required. For this reason Scheepers, Yang, Reuter and Adema (2006) proposed a Dynamic-CFD hybrid model, an architecture that employs a linear dynamic model structure as well as a CFD model structure. An adaptive, dynamic model in discrete time was chosen to model the system. The two classes of dynamic models chosen were (1) a *linear* model of the transfer function class with an auto-regressive exogenous (ARX) structure and (2) a *non-linear* model of the rule-based class. Owing to this fluctuating state in the furnace, the linear modelling technique had similar predictive abilities than the non-linear modelling technique. Subsequently, a linear model of the transfer function class and with an ARX structure was used to model the process.

**The key findings from the dynamic modelling** The ARX type linear, adaptive prediction model achieved an 8-hours-ahead predictive accuracy of 30% ($\pm$ 6% standard deviation) of future P$_2$O$_5$(slag) values. This 0.3 coefficient of determination
exists because, at the moment of any $P_2O_5(slag)$ prediction, the furnace contains metallurgical memory (data history) making sure that some predictive possibilities will always exist. Therefore, some of the historical data required for prediction are already in the furnace as a result of the 8-12 hours residence time.

C-fix and the silica gravel factor are independent variables used by operators to try and steer the process within a range of given setpoints. An ARX type linear, adaptive predictive control model utilising these two operator tool variables to simulate process control, achieved an 8-hours-ahead predictive accuracy of 35% ($\pm 7\%$). That is only a 5% improvement; the reason for this is that there exists a fundamental upper limit to predictive control improvement with the input variables assigned to facilitate process adjustments on a short term basis ($\leq 8$ hours) already in the furnace and no changes can be made to them.

**The CFD model development**  Complex process interactions in the furnace necessitated the creation of two process-specific, user-developed models that integrates accurate, thermodynamical data with computational fluid dynamics calculations, as well as reaction kinetics. (1) *The Reaction model* accounts for the downward flow of feed mixture and reduction of $P_2O_5$. It does this as a function of reaction kinetics and temperature, the subsequent creation of $P_4$ and CO from within the packed bed domain as well as the energy sinks due to phase transformation, heating, reaction and melting. (2) Thermal radiation within the packed bed is modelled by a *Particle-particle radiation model* that improves the gas phase radiation within the packed bed. It introduces particle-particle radiative aspects based on actual process conditions as a single, temperature-dependent effective thermal conductivity. The boundary conditions are provided by industrial measurements, and the key model parameters of reaction kinetics were obtained by laboratory experiments for different feed mixtures. The studied operating conditions include feed flowrate, bed porosity, reaction kinetics, $P_2O_5$ wt% in the pellets, electrode operating heights and individual electrode power. Outputs of the model are energy distribution within the packed bed, specific power consumption [MWatt consumed/ton $P_4$ produced], $P_2O_5$ wt% in the slag and off-gas gaseous temperature. Thirteen temperature probes installed inside the refractory lining of the furnace especially for this project allow parameter fitting and validation to be guided within the constraints of real measurements.

**The key findings from CFD modelling**  The most important finding of the CFD modelling was the existence of a narrow, gas-solid reduction zone where a very fast reaction takes place over a small temperature gradient. It is within this reduction zone that the bulk of the phosphorus is produced. The upper boundary of this reduction zone is mainly determined by the chemical composition of the pellet, bed conductivity and bed permeability i.e. the major variables controlling conduction and convection phenomena within the bed. The lower boundary of this reduction zone and therefore the thickness thereof, is mainly determined by the structural qualities of the sintered pellet, the porosity of the pellet and, to a lesser extent, the reaction rate kinetics. Above this reduction zone, evidence was found of a thermal reserve zone similar to the one found in an iron blast furnace. Fast reaction rates in combination with long residence times diminish the influence changing reaction
rates have on the process. Gaseous product and velocity information show low, recirculating gaseous flow velocity areas that cause dust accumulation, thus resulting in increased pressure measurement in the outlet duct. When, at a very late stage of the project, the finished model was presented with much more realistic electrode cooling water data (significantly different from the values used to construct the model) the model provided values closer to reality in three of the four major output variables. This concludes that the CFD model is robust, non-stiff (in a differential equation sense) and reflects reality.

**Fundamental design, sampling and process restriction** Both the dynamic model and the CFD model provided the same prognoses on general process trends and thereby validate the accuracy, as well as the legitimacy of the two modelling methods. However, fundamental design-, sampling- and process restrictions associated with the submerged arc furnaces limit the predictive and especially control accuracy or meaningfulness of the dynamic models. Prediction is only as good as the data it uses to generate that prediction! Therefore, these restrictions on good quality data also limit the accuracy of the CFD model. The point is made that, given the current status quo, no model can improve on an 8-hour-ahead prediction of 30% (6%). This barrier can only be pierced with e.g. tidier and more frequent sampling regimes and other upfront capital investments. Only once that is done, the vision for a better CFD model will become attainable. Such a decision becomes a cost analysis exercise and one that can only be taken at management level.
Samevatting

Het proces Het bestudeerde proces is de grootschalige productie van fosfor bij Thermphos International. De belangrijkste reactie is gedefinieerd in het Wöhler proces, waarbij een calciumsilicaat slak, calciumfluoride, koolstofmonoxide en het gewenste product, fosfor gas, geproduceerd wordt. De stroom grondstoffen, bestaande uit: gepelletiseerd apatiet, cokes en silicium (in de vorm van grind), worden gelijkmatig aan een submerged arc furnace toegevoegd, zodat een evenwijzig verdeeld gepakt bed met een constant volume verwezenlijkt kan worden. Het gasvormige product verlaat de oven door twee ventielen, die symmetrisch geplaatst zijn boven de ijzerfosfide aftap, in het dak van de oven. De ijzerfosfide wordt, normaal gesproken, een keer per dag afgetapt. De calciumsilicaat slak wordt echter continu afgetapt via twee alternerende, watergekoelde tapgaten, die zich op 400 mm boven de ovenvloer bevinden. Vanwege de grote slakproductie, zal een geringe hoeveelheid P\(_2\)O\(_5\) wt% in de slak (P\(_2\)O\(_5\)(slag)) reeds resulteren in een substantieel verlies van ongereducede, potentieel product.

Controle Het controleren van het proces, om de hoeveelheid P\(_2\)O\(_5\)(slag) zo laag mogelijk te houden, is daarom een van de belangrijkste prioriteiten. Dit is de reden voor de keuze van P\(_2\)O\(_5\)(slag) als de belangrijkste output variabele in de opgestelde modellen. Het ovenproces wordt automatisch geregeld door de stroom constant te houden, wat mogelijk is door de hoogte van de elektoden aan te passen. Afgezien van automatische controle, kunnen de mengverhoudingen van fixed carbon-to-P\(_2\)O\(_5\) (C-fix), silica gravel-to-pellets (silica gravel factor) en coke-to-pellets (coke factor) dienen als volledig onafhankelijke variabelen, die door de procesoperator gebruikt kunnen worden om het proces te sturen en te optimaliseren. Om de kwantitatieve invloed van deze en meer afhankelijke variabelen beter te begrijpen, is ruwe industriële data bestudeerd. Een veel gebruikte oplossing in de fosforindustrie om voor hoogge P\(_2\)O\(_5\)(slag) te compenseren is het verhogen van C-fix in het gepakte bed, met als resultaat een lagere hoeveelheid P\(_2\)O\(_5\)(slag) vanwege extra reductie door de toegevoegde cokes. Het is echter bewezen dat deze oplossing, die breed wordt gedragen, niet altijd het gewenste resultaat oplevert. Bij constante Moeller flowrates, is de P\(_2\)O\(_5\)(slag) waarde vrijwel onafhankelijk van C-fix en voornamelijk een functie van de verblijftijd van de grondstoffen in de oven.

Dataverwerking en optimale procesoperatie limieten Vanwege het feit dat slak-, ijzerfosfide- en P\(_4\) flowrates niet direct gemeten worden, is de dataverwerking opgebouwd rond een van de ovens gedurende een periode van zes maanden. Zo
zijn real-time flowrates verkregen, die soft-sensor waarden leveren. Deze waarden zijn gebruikt in een berekening van de proceskosten, waarbij blijkt dat de meest winstgevende situatie ontstaat als met Moeller flowrates van $\geq 25-30 \text{ [ton/hour]}$ en C-fix $\leq 0.475$ gewerkt wordt. Dit is echter het gebied met de hoogste hoeveelheid $P_2O_5(slag)$, dus afnemende elektriciteitskosten en niet de afnemende hoeveelheid $P_2O_5(slag)$ geven daarbij de doorslag. Dit toont aan dat het streven naar een lager SPC de meeste winst oplevert en niet het streven naar een hogere $P_4$ opbrengst.

Een dynamisch CFD hybride model Een fosfor producerend submerged arc furnace fluctueert continu tussen de dynamisch gedreven en de thermodynamisch bedreven modus. Hierdoor kan het proces niet via één enkel model beschreven worden en is het erg lastig om via de standaard software die gebruikt wordt voor kinetisch en thermodynamisch modelleren een betrouwbare model op te stellen, dat het dynamische proces goed weergeeft (Reuter and Yang, 2005). Een combinatie van modelleren technieken is daarom vereist. Daarom is een Scheepers, Yang, Reuter and Adema (2006) dynamisch CFD hybride model voorgesteld met een structuur die zowel een lineair dynamisch model als een CFD model behelst. Een aanpasbaar, dynamisch model in discrete tijd is gekozen om het systeem te modelleren. De twee gekozen methoden voor het dynamisch modelleren zijn (1) een linear model van de transfer function class met een auto-regressive exogenous (ARX) structuur en (2) een non-linear model van de rule-based class. Vanwege de fluctuerende modus in de oven, hebben zowel de lineaire- als de niet-lineaire modelleringtechniek gelijkwaardige mogelijkheden het proces te voorspellen. Daarom is ook een lineair model van de transfer function class met een ARX structuur opgesteld om het proces te modelleren.

De belangrijkste waarnemingen uit het dynamisch modelleren Het lineaire aanpasbare ARX type model behaalde bij een voorspelling van 8 uur vooruit een betrouwbaarheid van 30% ($\pm 6\%$ standard deviatie) voor $P_2O_5(slag)$ waarden. Deze 0.3 coëfficiënt is aanwezig omdat, op het moment van elke $P_2O_5(slag)$ voorspelling, het geheugen effect van de oven er voor zorgt dat sommige voorspelde mogelijkheden altijd kunnen voorkomen. Dus sommige historische data, die nodig zijn voor de voorspelling, bevindt zich al in de oven vanwege de verblijfstijd van 8-12 uur. C-fix en de silica gravel factor zijn onafhankelijke variabelen, die gebruikt worden door operators om het proces binnen bepaalde limieten te kunnen sturen. Een lineair aanpasbaar ARX type model, dat gebruik maakt van deze 2 variabelen om het proces te simuleren, behaalde bij een voorspelling van 8 uur vooruit een betrouwbaarheid van 35% ($\pm 7\%$). Dit is slechts een verbetering van 5%. De reden hiervoor is de theoretische bovenlimiet van het voorspellen van verbetering met de gebruikte variabelen, die bedoeld zijn voor snelle aanpassing van het proces, ($\leq 8$ hours) already in de oven en deze kunnen niet aangepast worden tijdens het proces.

De ontwikkeling van het CFD model De complexe processen in de oven hebben er toe geleid dat het noodzakelijk was om twee modellen op te stellen, die zowel accurate, thermodynamische data met computational fluid dynamics als
The Reaction model beschrijft de afname van de toegevoegde grondstoffen en reductie van P\textsubscript{2}O\textsubscript{5}. Deze afname is beschreven als functie van reactiekinetiek en temperatuur, zowel de vorming van P\textsubscript{4} en CO vanuit het gepakte bed en de energieconsumptie nemen af van wege verhitting, reactie en smelten. (2) Thermische straling in het gepakte bed is gemodelleerd via Particle-particle radiation model dat de gasfase straling in het packed bed verbeterd weergeeft. Het introduceert stralingsinteractie tussen deeltjes, gebaseerd op actuele procescondities als zelfstandige, temperatuurafhankelijke effectieve thermische geleiding. De limieten komen uit industriële metingen en de belangrijkste parameters voor reactie kinetiek zijn verkregen via laboratorium experimenten aan verschillende grondstoffen mengsels. De bestudeerde bedrijfscondities zijn: toevoegsnelheid van grondstoffen, porositeit van het packed bed, reactiekinetiek, P\textsubscript{2}O\textsubscript{5} wt% in de pellets, elektrodehoogte en de stroom over de individuele elektrodes. De output van het model omvat energiespreiding in het gepakte bed, specifieke elektriciteitsconsumptie [MWatt opgenomen/ton P\textsubscript{4} geproduceerd], P\textsubscript{2}O\textsubscript{5(slak)} en off-gas temperatuur. Der- tien temperatuursensoren, die speciaal voor dit project geinstalleerd waren in de ovenwand, zorgen ervoor dat parameterfitting en controle binnen de limieten van reële metingen blijven.

De belangrijkste waarnemingen uit het CFD modelleren

De belangrijkste waarneming van het CFD modelleren is de aanwezigheid van een smalle gas-solid reductiezone, waarin een zeer snelle reactie plaatsvindt in een kleine temperatuursgradient. Het is in deze reductiezone dat de overgrote hoeveelheid van de fosfor wordt gevormd. De bovenlimiet van deze reductiezone wordt voornamelijk bepaald door de chemische samenstelling van de pellets, geleiding in het bed en permeabiliteit van het bed dus eigenlijk de belangrijkste variabelen die geleiding- en convectie processen in het bed reguleren. De onderlimiet van deze zone, die tevens de dikte van de zone bepaalt, wordt voornamelijk bepaald door de structurele eigenschappen van de gesinterde pellet, de porositeit van de pellet en in mindere mate door de reactiekinetiek. Boven deze reductiezone is bewijs gevonden van een thermal reserve zone, zoals deze ook in een hoogoven worden aangetroffen. Snelle reacties in combinatie met lange verblijfstijden, verminderen de invloed, die veranderende reactiesnelheden hebben op het proces. Informatie over de circulatie van gasvormig product, toont aan dat er zich in de oven gebieden bevinden met een lagere circulatiesnelheid, waardoor stofophoping kan optreden, wat weer tot verhoogde drukmetingen in de outlet leidt. Toen, in een erg laat stadium van het project, betere koelwaterdata van de elektroden beschikbaar kwamen (significant verschillend van de data gebruikt voor het opstellen van het model), bleek dat het model voor drie van de vier belangrijkste output variabelen waarden gaf, die veel dichter bij de realiteit lagen, Dit bewijst dat het CFD model robuust, dynamisch (als in een differentiaal vergelijking) en realiteitsgetrouw is.

Fundamenteel ontwerp, monstername en proces restricties

Zowel het dynamisch- als het CFD model geven dezelfde prognose, als algemene procestrends beschouwd worden, en daarmee onderschrijven ze de nauwkeurigheid en de correcte keuze van de twee modelleringsmethoden. Of dynamische modellen zinvol zijn, wordt
echter bepaald door fundamentele ontwerp-, monstername- en procesrestricties, behorende bij submerged arc furnaces, die de nauwkeurigheid van de voorspelling en de controle hierover beperken. Een voorspelling is zo goed als de data die gebruikt zijn voor die voorspelling! Daarom beperken deze restricties ook de betrouwbaarheid van het CFD model, zelfs als data van goede kwaliteit gebruikt worden. De conclusie is, gezien de huidige omstandigheden, dat er geen model is om de voorspelling van 8 uur vooruit van 30% (6%) te verbeteren. Deze barrière kan alleen bereikt worden door bv. een betere en frequentere monstername en andere kapitaal investeringen. Slechts als aan deze voorwaarden is voldaan, zal de visie van een beter CFD model in zicht komen. Deze besluitvorming is onderhevig aan financiële mogelijkheden en zal daarom op management niveau genomen dienen te worden.
Chapter 1

Introduction

Pyrometallurgical operations, such as those occurring in bath type smelting- or reduction furnaces, seldom lend themselves to accurate characterisation, unlike processes occurring at lower temperatures and less aggressive chemical conditions. Measurements of temperature, liquid level, pressure and flow rates, which often are trivial at lower temperatures are either not possible or can simply not be determined at higher temperatures. These practical limitations constrain furnace controllability, especially with conventional methods associated with other, low temperature processes. Most furnaces are operated in a semi-batch way and operate with medium to large inventories and the residence times and process time constants are long. These controllability-issues imply that good feedforward models becomes very important for proper control, as the cost of rectifying upset conditions are so significant. Traditionally furnace control is either experience based (with the expert device depending on the expert observer), or it is based on either a totally empirical approach, or on a thermochemical mass and energy balance model. The empirical approach very often provides short term accuracy, but only until some fundamental shift in operating conditions occurs. On the other hand, fundamental approaches are seldom of acceptable accuracy for the purpose of control. They do, however, give some insight into the process phenomena. As feedback-control for these furnaces is technically not feasible and unstable, one has to rely on control which combines the qualities of fundamental predictive models with the empirical models and computational fluid dynamics (Eksteen, 2004).

1.1 Research motivation

A project was initiated that would attempt to increase the understanding of all the complex interactive processes inside a phosphorus producing submerged arc furnace and thereby provide industry with relevant information and tools to decrease the specific power consumption (SPC) \( \text{tonP} / \text{MegaWatt} \) and increase profitability. A submerged arc furnace, however, is a very complex system in both physical and chemical aspects. It involves multi-phase, high temperature reduction reactions, energy conversion and distribution from electric power through arcs and conduction. Although the underlying chemical reaction and to a lesser extent the kinetics
driving the main reactions in the submerged arc furnace are well documented, it is the complex interaction between these phenomena and the intricate burden characteristics influencing the ohmic resistance of the feed material that cause the specific power consumption (the energy consumed for every ton of \( P_4 \) produced) to be an uncontrollable, dependent variable. Above all others, the specific power consumption is the most symptomatic indication of the profitability of the process and the optimisation thereof a top priority at any phosphorus producing company.

This project is a venture between the Prof. Markus Reuter, Delft University of Technology, SenterNovem and Thermphos International, a large-scale, phosphorus producing company situated in Vlissingen, The Netherlands.

1.2 The process in brief

The process under investigation is the large-scale production of phosphorus at Thermphos International. The main reaction as defined by the Wöhler process (Corbridge, 1995) proceeds according to Equation 1.1. From pelletised (fluoro)apatite (\( \text{Ca}_{10}(\text{PO}_4)_6\text{F}_2 \)), coke and silica (in the form of gravel). It produces a calcium-silicate slag, calcium fluoride, carbon monoxide and the desired product, phosphorus gas.

\[
\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2 + 15\text{C} + 9\text{SiO}_2 \rightarrow 3\text{P}_2(\text{g}) + 9[(\text{CaO} \cdot \text{SiO}_2)] + \text{CaF}_2 + 15\text{CO}(\text{g})
\] (1.1)

Gravity delivers the feed to the submerged arc furnace through ten, evenly distributed feed chutes ensuring constant packed bed volume (see Figure 1.1). The gaseous product leaves the furnace through two symmetrically spaced outlet vents situated above the ferrophosphorus tap hole in the roof of the furnace. The ferrophosphorus is tapped off, usually once per day. Slag, however, is continuously tapped through two alternating, water-cooled tap holes located 400 mm above the furnace floor. Owing to the large production volume of slag, a seemingly small amount of \( \text{P}_2\text{O}_5(\text{slag}) \) results in substantial losses of unreduced, potential product. Controlling the process in order to keep the \( \text{P}_2\text{O}_5(\text{slag}) \) as low as possible, is therefore another top priority.

1.3 Research focus area

The feed material forms the major resistance of the smelting furnace circuit. As the feed materials descend towards the hot zone in the furnace, the feed material starts to soften and melt, significantly lowering the electrical resistance. A conductive path is thus provided between the electrodes where the \( \text{I}^2\text{R} \) or the Ohmic energy is released to attain the high temperatures and energy levels necessary to effect the endothermic reactions. These reactions take place in a domed-shape area, or reduction zone around the tips of the electrodes. The directional distribution of this ohmic energy and the shape, size and reach of this reduction zone through the packed
1.4 Research objectives

Following from the motivation and process phenomena previously discussed the following project objectives were identified:

1. Perform a data mining exercise on the three Thermphos International furnaces, utilising three years of industrial data. Investigate the influence of various fixed carbon-to-\(P_2O_5\) ratios on the loss of potential product in the slag phase, the influence of overall feed flowrate (related to the residence time in the furnace) on the specific power consumption and the recovery and the optimum
Introduction

conditions conducive to profit making. Perform a mineralogical dig-out of the inside of a furnace as well as a slag sample campaign on an operating furnace.

2. Reconcile relevant industrial data and perform a cost analysis study. Owing to the fact that the slag-, ferrophosphorus- and P\(_4\) flowrates are not directly measured at each individual furnace and are needed for the cost analysis exercise, data reconciliation is necessary to obtain these flowrates in a real-time way. Data reconciliation also prepares the data for further dynamic modelling.

3. Use intelligently structured data in order to investigate the continuous state of the submerged arc furnace process. These findings would shed light on which type and class of model could best describe the process.

4. Develop a linear, adaptive predictive model utilising the autoregressive, exoge-

    neous input transfer function structure in order to predict the P\(_2\)O\(_5\)(slag) up to 8 hours in the future. Quantify the influence of all dependent and independent input variables on the process.

5. Construct, test and validate an array of steady-state, computational fluid dy-

    namics (CFD) models corresponding with a range of industrial process condi-

    tions. These models would validate data-mining findings and provide a virtual window to the inside of the furnace to give the operators an idea of the changing conditions inside the furnace. Complex, user-developed sub-models will be utilised.

6. Use the predictive abilities of both the above-mentioned models and unify-

    ing them into one single modelling approach called a dynamic-CFD hybrid model that would increase prediction, increase understanding of the process and optimise process control.

1.5 Research contributions

The following are the contributions of this research:

- It introduces a conceptual framework of a Dynamic-CFD hybrid model that utilises both the robust functionalities of linear modelling techniques in combination with the intricate solving capabilities of computational fluid dynamics. This architecture is new.

- A thorough data mining exercise of the process that highlights the asymmet-

    rical nature of this submerged arc furnace and understanding of how such behaviour can be minimised and utilised in modelling.

- A structure for reconciling process data within their inherent limitations, utilising the soft-sensing power contained within the method. Simple cost analysis procedures using these soft sensor values to determined the operating range of maximum profitability.
1.5 Research contributions

- Proof that the submerged arc furnace is continuously fluctuating back-and-forth between a flowrate(dynamically)-driven state and a composition(thermodynamically)-driven state. It is owing to this fluctuating state in the furnace that linear modelling techniques provide similar predictive abilities than non-linear techniques.

- A linear, adaptive prediction model with an auto-regressive, exogenous input structure (ARX) that predicts P$_2$O$_5$ wt% values in the slag for 8 hours in the future.

- A phosphorus producing, submerged arc furnace CFD model developed in which fluid flow and energy distribution as a function of chemical reactions, heating of material and cooling losses are simulated in a fully 3-D way. The complexity of the process necessitated the development of two user-developed models. The Reaction Model simultaneously accounts for the depletion of P$_2$O$_5$, the formation of the gaseous product as well as the energy exchanges associated with the chemical reactions and the heating and melting of a heterogeneous packed bed burden, through the unique introduction of an user-developed, effective heat capacity equation. The Particle-particle radiation and effective thermal conductivity Model improves the Porous Media model’s predictive accuracy at high temperatures by incorporating both conductive, as well as particle-particle radiative aspects based on actual process conditions into the model as a single, temperature-dependent effective thermal conductivity value.

- It highlights that the integration of accurate, multi-field thermodynamical data with computational flow dynamics was successful, further unifying the sciences of kinetics and equilibrium thermodynamics. An extensive and methodical validation campaign that ensures industrially endorsed results. Figure 1.2 shows (from left to right) A. Adema, the author and Y. Yang at a routine furnace shutdown ready to extract the mineralogical samples. The pictures were taken by Prof. M. A. Reuter.

- It shows that the obtainable accuracy of both model is limited by fundamental design-, sampling- and process restrictions associated with the production of phosphorus with submerged arc furnaces and that improved prediction can only come from capital investment.

**Referred journal articles**


**Conference articles**


**Reports to SenterNovem**


### 1.6 Outline of the thesis

The remainder of this thesis is divided into three parts and 11 chapters.

**Part I** lays out how phosphorus is produced by using a submerged arc furnace. It tracks the feed material from storage into the heart of the furnace, describes the furnace itself and follows the path of all the product streams. It explains the role of the Moeller resistance as part of the electrical circuit and breaks down the constant-current principle that controls the furnace process. Finally, it describes the tools that are available for the operators to steer the process in order to maximise production and minimise cost. It lays out how phosphorus is produced by using a submerged arc furnace. It shows the reality of asymmetrical furnace operation that culminates in lopsided erosion patterns. It comments on the data that highlight the practical aspect of every day process fluctuations and problems that included Moeller collapses and unequal tapping ratios. It shows the standard deviation within a single
sample of an important setpoint value and demonstrates the diverse mineralogy of furnace-lining samples obtained from a dedicated sampling campaign. Finally, a short introduction is given about the potential of such asymmetrical behaviour and its corresponding variables to play a role in the development of Dynamic and CFD models.

**Part II** explains how the submerged arc-furnace is continuously fluctuating between the dynamic-driven- and thermodynamic-driven state and how one single modelling approach can not be sufficient. In light of this the Dynamic-CFD hybrid model is proposed.

**Part III** starts by investigating raw Thermphos International industrial data. The data are then reconciled (the first step towards the development of a dynamic predictive model) because a significant degree of uncertainty can be associated with industrial data. Finally, a minimal furnace operating cost analysis exercise is performed. Unified and comprehensive coverage of the principles, perspectives and methods of adaptive prediction is provided. It describes the prediction and predictive control problems and how they are relevant to the Thermphos International situation. The furnace’s perpetual fluctuation between a dynamic-driven state and a thermodynamic-driven state is demonstrated and the concepts explained. A special feature is the comparison made between linear and non-linear dynamic models while using the same data. It continues by making an informed choice between these two modelling methods. The history of data is discussed and it is shown how the ARX structure model can accommodate the “metallurgical memory” of the furnace in order to improve prediction. By assuming future values of the two variables deemed operator’s tools, predictive control is simulated in another section. Part III finishes with a sober assessment of the possibilities for prediction and predictive control given certain fundamental design-, sampling- and process restrictions associated with the production of phosphorus with submerged arc furnaces.

**Part IV** discusses the theory and methodology involved in CFD process modelling. Fundamentals are introduced and discussed and steps required in building a CFD model are given. The development of a CFD model for the submerged arc furnace is described. The assumptions and simplifications, the selection of the physical models and model parameters and the details of the development of user sub-models are discussed in detail. The heating and melting process, the chemical reactions, the creation of mass, the introduction of energy to the furnace and temperature dependent effective thermal conductivity were simulated with two user-developed sub-models. A base case data scenario is used to generate general results that are presented in a graphical manner. Based on the developed CFD model, some sensitivity analyses were carried out and process improvement and optimization concepts were discussed based on the modelling results.
Part I

The PRODUCTION of PHOSPHORUS
Chapter 2

The phosphorus production process description

There is distinct reduction zone in the descending packed bed where the gaseous product is optimally generated. This reduction zone is greatly influenced by the residence time of the feed material inside the furnace. Residence time is not a directly adjustable variable but is dependent on a large amount of interconnected and interactive variables. However, residence time is the most influential variable when looking to control the process. One of the few independent variables available to operators is the ratio of fixed carbon-to-$\text{P}_2\text{O}_5$ addition. In order to better understand this variable and its link to residence time and control, the phosphorous producing process is explained in some detail. In a wider sense, there exists an ever-pressing need to better comprehend the closure of elemental loops within, not only a furnace, but in the environment as a whole. This is particular true for the phosphorus loop. With a future where more and more secondary, recycled feed materials (e.g. chicken manure) will be utilised as reactants, the need to better control the process in order to ensure sustainable phosphorus production as well as an environmentally sound society, will increase. The data reported on were all measured by the author and interpreted in the context of this thesis.
2.1 Furnace modelling and control in the context of sustainable resource processing and recovery

Reactors like the submerged arc furnace under investigation, constitute a key processing component in the total primary and secondary resource cycle, as the furnaces perform not only primary operations, but also more and more secondary operations. To control the overall resource cycle effectively, one needs to take a systems modelling approach of the whole cycle, seeking to understand the dynamic process behaviour of the individual components of the cycle, and then specifically the part that contribute most to the chemical conversion, namely the pyrometallurgical reactor or furnace. Metals and products like phosphorus are produced through a long chain of processes. For primary resources, valuable material production proceeds via mining, mineral processing, ore smelting, conversion and refining steps of via hydrometallurgical processes, or a combination of pyro- and hydrometallurgy. For secondary resources, metals are separated and recovered from a diverse range of materials, which play an increasingly important role in the world. After metal extraction, either from primary or secondary resources, the crude product have to be further refined or manufactured into various types of by-products and finally shaped into different products to the end-users. Since the end-user eventually discards these products, the contained metals and products like phosphorus find their way back into the resource cycle as scrap. Therefore, good metallurgical reactor control implies improved control of the material quality in the metals cycle, from production to the end-use, up to the recycling phase. This implies that the metallurgical processes in each unit operation in the metals production and processing chain have to be controlled, so as to achieve optimal performance of high product quality, low energy and materials consumption and low environmental impact (Eksteen, 2004).

Sustainable processing is not possible without proper reconciled material flow models and proper dynamic process models that can be used to manage or control processes. The objectives of these control actions are very clear; they should optimise product quality, minimise energy consumption and optimise product flow. Therefore, control should not only maximise economical benefits, but at the same time also minimise associated ecological effects (Reuter et al., 2005). Despite the above-mentioned ideals for process modelling and control of reactors like submerged arc furnaces, actual model-based control of process metallurgy in furnaces remain elusive. The model presented in this study provides a few more additional steps in a journey of a thousand miles.

2.2 The importance of the reduction zone

At the top of the charge (top of the packed bed) in the furnace only solid pellets, coke particles and silica gravel are present (see Figure 1.1). As the feed materials descend towards the hot zone in the furnace around the electrodes, the critical temperature of about 1150°C will see the onset of reduction reactions and the subsequent
2.3 The concept of residence time and its role in furnace control

When operators make adjustments to the recipe of the feed material, the new mixture will not immediately influence the process. The new mixture will first make its way down the feed chutes, enter the furnace, slowly descend with the charge until it finally reaches the reduction zone, partake in the Wöhler (and other reactions) and then exit the furnace. It is only during these last phases of its journey that the new mixture will effect any of the correcting changes it was originally intended for. The time it takes for this mixture (input variable(s)) to eventually exit the furnace is, in the context of this study, called the total residence time \( (\tau_{\text{tot}}) \). Total residence time can loosely be translated as:

**Figure 2.1:** An illustration of the domed-shaped reductive zone in the packed bed as predicted by the CFD model of the author.
1. the time from when the adjusted (new) Moeller feed mixture (changed at the weighing stations) enters the feed chutes situated above the furnace until it enters the furnace, $\tau_{\text{feedchutes}}$, plus

2. the time from the top of the packed Moeller bed in the furnace until it reaches the reduction zone (see Section 2.2), $\tau_{\text{beforeRZ}}$, plus

3. the time it takes from the reduction zone until the (now melted) new feed mixture (or imaginary trace element) exits the furnace as slag, $\tau_{\text{afterRZ}}$.

$$\tau_{\text{tot}} = \tau_{\text{feedchutes}} + \tau_{\text{beforeRZ}} + \tau_{\text{afterRZ}}$$

$$\tau_{\text{tot}} = (1 - 2 \text{ hours}) + (6 - 8 \text{ hours}) + (1 - 2 \text{ hours}) = 8 - 12 \text{ hours}$$

with $\tau_{\text{furnace}} = \tau_{\text{beforeRZ}} + \tau_{\text{afterRZ}}$ (2.2)

In a mathematical sense, the residence time is similar to a time constant. The time constant is used to tell in which time scale any output changes and then approaches the unit step value in response to a step response (Ljung, 1994). The step response of a dynamical system consists of the time (time constant) behaviour of its outputs when its control inputs are unit step functions (a discontinuous function whose value is zero for negative argument and one for positive argument) (Kanjilal, 1995), for a given initial state. In control theory, step response is the time behaviour of the outputs of a general system when its inputs change from 0 to unity value in a very short time. In the case of Thermphos International, this input change in a very short time, or unit step, represents the feed adjustments, while the unit step response value represents the influence these adjustments have on the output.

Constant current control principle

Figure 2.2: A graphical depiction of the dependence architecture of the residence time, illustrating its complete dependence on a vast array of different variables.
2.4 Introduction to the phosphorus producing process

It is important to understand that the residence time is not a directly adjustable variable. The residence time is dependent on a large array of interconnected and interactive variables. This principle is illustrated in Figure 2.2.

- \( \tau_{\text{tot}} = \text{function} \) (Moeller flowrate, heap density of packed bed, porosity, freezeline, packed bed volume)

- \( m_{\text{Moeller}} = \text{function} \) (megaWatts consumed in the furnace [MW])

- \( MW = \text{function} \) (packed bed resistance [mΩ], electrode operating heights)

- \( m\Omega = \text{function} \) (packed bed homogeneity)

- Packed bed homogeneity = \( \text{function} \) (1. Size, shape and density of particles, 2. Solid flow characteristics, 3. Thermodynamics and kinetics, 4. operator tools)

It is shown that \( \tau_{\text{tot}} \) inside the furnace is a dependent variable and a function of a series of different parameters and can not simply be adjusted. The key is to focus on the independent input variables, or operator tools shown in Figure 2.2 that can be controlled and investigate in which way they can effectively influence the process. The most important of these will proof to be the C-fix ratio. With \( \tau_{\text{tot}} \) and C-fix shown to be ultimately interrelated, C-fix represents a clearly defined independent variable subject to operators input from the control room that could be manipulated in order to optimise the process. Large portion of this study is therefore dedicated to looking into the relationship between these two variables and the influence that changes in the C-fix ratio has on the residence time and the process output. In order to provide the reader with a more complete picture of these (C-fix and \( \tau_{\text{tot}} \)) and other concepts (e.g. the ratio of silica gravel-to-pellets addition) the full phosphorus producing process is described in detail.

2.4 Introduction to the phosphorus producing process

The Company

Thermphos International produces and sells phosphorus and phosphorus derivatives. These products are used as base materials in for example pharmaceutical products, foodstuffs, crop-protection agents and industrial and household cleaning products. Thermphos International’s principal place of business is in Vlissingen, The Netherlands, where it employs about 450 people (ThermPhos International Website, 2003). Thermphos International produces about 80000 tons of phosphorus per year. Other production outputs include 550000 tons of calcium silicate slag, 200000 tons of CO gas and 5000 tons of ferrophosphorus, all calculated on a yearly basis.

The Element

About 100 years ago three major allotropic modifications of elemental phosphorus had been generally recognised; white (or yellow when impure), red and black. In
addition, gaseous and liquid states, and many other solid forms of the element are now known, although most of the latter can be regarded as sub-varieties of the three main allotropes. White phosphorus, the longest known form, is the most volatile and reactive form of the solid, and is closely related to the liquid and vapour phases of the element into which it readily transforms. Its molecular weight in solvents corresponds to $P_4$, as it is in the liquid and vapour states. Solid white phosphorus is a soft and waxy substance with a density of 1830 kg/m$^3$ at 20°C, a melting point of 44°C and a boiling point of 280°C. White phosphorus is virtually insoluble in water ($\leq 0.0005\%$) and it can be stored, fused and transported quite safely under an aqueous layer. At about 30°C, however, water does dissolve in white phosphorus to the extent of 0.1 mg/g of $P_4$. If it is exposed to both air and water, under conditions in which it will not inflame, a complex mixture of oxyacids is slowly produced (Corbridge, 1995).

**Phosphate recovery**

Phosphates could be recovered from several sources; sewage, animal manure, animal bones and waste streams from different industrial processes (e.g. food industry, metal treatment industry). The main focus and research is on phosphate recovery from sewage and animal manure. Phosphates in sewage originate from human excreta and detergents, at an estimated rate of 2.5 g P per person per day. In the Netherlands this corresponds to 14600 tons P per year; at an estimated recovery rate of 83%, 12000 tons P is available for recovery from sewage sludge (Stark, 2005). The EU Urban Waste Water Treatment Directive 91/271 and the Water Framework Directive 2000/60 requires that phosphates (from human, animal, detergent or industrial origin) are transferred into sewage or collected animal manures. This will prevent eutrophication of surface water by the phosphates. Eutrophication is the excessive growth of vegetation, algae, due to the high nutritional value of phosphorus causing a strong reduction in oxygen levels in the water as well as blocking sunlight. Phosphorus in surface water originates from several sources as shown in Table 2.1.

**Table 2.1:** Phosphate sources in surface water (*CEEP (Centre European Etudes des Polyphosphates), 2005*).

<table>
<thead>
<tr>
<th>Type</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sewage</td>
<td>34%</td>
</tr>
<tr>
<td>Human source</td>
<td>14%</td>
</tr>
<tr>
<td>Detergents</td>
<td>24%</td>
</tr>
<tr>
<td>Livestock</td>
<td>34%</td>
</tr>
<tr>
<td>Industry</td>
<td>7%</td>
</tr>
<tr>
<td>Fertiliser</td>
<td>16%</td>
</tr>
<tr>
<td>Background source</td>
<td>9%</td>
</tr>
</tbody>
</table>

The Institute for European Environmental Policy estimated that this will result in 220000 - 240000 tons per year of phosphates being transferred into sewage sludge. Around 2 million tons per year of phosphates are present in agricultural manures. Currently in Europe 53% of sewage sludge and the majority of animal wastes are spread on agricultural land. Agricultural spreading of sewage sludge is however be-
coming less of an option and has completely disappeared in some countries. Logistic, environmental and fears over contamination are becoming major obstacles. In the Netherlands, due to the large amount of livestock, agricultural spreading of animal manure is also restricted. In combination with fertilisers the spread manure contains more phosphates and nitrates than the soil can handle. Landfill of untreated sludge as well as sea dumping is no longer allowed in Europe. Sludge treatment and disposal is now the highest operating cost factor for sewage works. Phosphorus recovery from sewage sludge will improve sludge management. It reduces the quantity and the phosphate content of sewage sludge, improving its characteristics for further processing. Thermphos International has examined the feasibility of recovering phosphates from sewage sludge or sludge incineration ash containing approximately 7% phosphorus. High levels of iron, copper and zinc present cause the sludge to be incompatible with the Thermphos International process. However, if phosphate is recovered by a precipitation process within the sewage works (as calcium or aluminium phosphates) these levels are significantly lower and problems are avoided. This is being done by Thermphos International for some years now, processing calcium phosphates recovered from a water treatment plant. Another source of phosphorus recently used is precipitated K-struvite (potassium magnesium phosphate) from a calf manure treatment installation. A year’s production of the installation can be processed in 4 days as 3% of the feed. The magnesium improves slag characteristics and the potassium does not pose any problems at this levels. Experiments were also conducted on the processing of finely ground bones, so-called bone meal. The use of secondary feed materials at Thermphos International such as sewage sludge, animal manure or bone meal instead of primary ores agrees with the basic notions of Industrial Ecology. The use of recovered phosphates connects the industrial phosphorus production process with its surroundings, in this case quite literally an ecosystem. It optimises a material cycle by reverting from limited ores to limitless waste supply. (Phosphorous recovery, 2001) (University, 2004)

2.5 The reduction of phosphorus according to the Wöhler reaction

Large-scale production of phosphorus uses the Wöhler process, in which apatites (nearly always fluorapatite) are reduced in the presence of carbon (coke) and silica (gravel) in submerged electric arc furnaces at temperature of between 1150 and 1400°C. The reaction proceeds according to the Equation 2.3,

\[
\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2 + 15\text{C} + 9\text{SiO}_2 \rightarrow 3\text{P}_2(\text{g}) \\
+9[(\text{CaO} \cdot \text{SiO}_2)] + \text{CaF}_2 + 15\text{CO}(\text{g})
\] (2.3)

thereby producing a liquid calcium silicates slag, calcium fluoride, carbon monoxide gas and the desired product, phosphorus gas. The reaction equation used in this thesis is simplified to the reaction mechanism of pure tricalciumphosphate.
The process has intermediate reactions and in practice the phosphate rock will always have some impurities, with one of the most important being iron oxide, which will be reduced and form iron phosphides, resulting in a second liquid product, namely ferrophosphorus. Iron is undesirable because it requires additional carbon and power for reduction and it locks up a certain percentage of phosphorus. Other impurities include alumina which increases the slag bulk but reduces the melting point somewhat. Fluorine is almost always present and is partly evolved as a gaseous compound (e.g. SiF$_4$). The balance finds its way into the slag (probably) as CaF$_2$. The phosphate can also contain some excess lime and/or magnesia over and above that required to form trivalent phosphates. White (and yellow when impure) ignites spontaneously in air at room temperature and is, therefore, conveniently handled under hot water at a temperature of 55 to 60°C when it will flow freely and can be pumped. It has a s.g. of slightly over 1700kg/m$^3$ just above its melting point when saturated with water.

### 2.6 Feed material

The four basic materials required for the production of phosphorus are coke (and/or antracite), silica (in the form of gravel), slurry and phosphate ore.

#### 2.6.1 Coke

In general, dried metallurgical coke is used. The maximum moisture content in the coke should ideally be less than 1% and it is therefore dried in a Lepol roaster before being fed to the furnace. All raw materials should be dry because the presence of moisture consumes not only power but also carbon.

\[
\text{H}_2\text{O}_g + \text{C}(s) \rightarrow \text{CO}(g) + \text{H}_2(g) \\
\text{with } \Delta G = 39 \text{ kJ (at 400°C)}
\]

The coke particles are also crushed and screened, thereby ensuring that overly small particles, as well as coke dust do not enter the furnace. Trouble-free operation of a phosphorus furnace requires that the raw materials should be more or less devoid of small particles and dust particles, so that the solid burden in the furnace has relatively constant gas permeability throughout its volume. The reaction gases, phosphorus and CO$_2$, formed in the lower part of the furnace, should also give up as much of their heat as possible to the burden as they pass through the bed. This movement of gases should be accompanied by as few pressure fluctuations as possible. High dust content in the burden will therefore lead to blockages in the burden bed and consequent pressure surges and temperature peaks.
2.6 Feed material

Table 2.2: The average composition of coke used at Thermphos International

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed carbon (C)</td>
<td>90%</td>
</tr>
<tr>
<td>SiO₂</td>
<td>8%</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>1%</td>
</tr>
<tr>
<td>Other volatiles</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

It is possible to replace a large proportion of this coke by cheaper petroleum coke. In this case, a higher proportion of organic impurities in the phosphorus must be accepted.

2.6.2 Silica gravel

Industrial sand and gravel, often called "silica," "silica sand," "silica gravel" and "quartz sand," includes sands and gravels with high silicon dioxide (SiO₂) content. Deposits of this silica gravel containing more than 97% SiO₂ are fairly common but not every phosphorus installation has such a deposit in the vicinity. Either higher costs of transporting the silica would have to be incurred, or the disadvantages of lower quality silica (high impurity levels, especially Fe₂O₃) would have to be tolerated. Thermphos International does not screen or dry the silica gravel before utilisation.

Table 2.3: The average composition of silica gravel used at Thermphos International

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>95%</td>
</tr>
<tr>
<td>CaO</td>
<td>4%</td>
</tr>
<tr>
<td>MgO</td>
<td>0.5%</td>
</tr>
<tr>
<td>Other</td>
<td>0.5%</td>
</tr>
</tbody>
</table>

2.6.3 Slurry

The slurry is a mixture of clay, water, Cottrell dust, Rotschlamm, STPP and Dorrschlamm.

- Cottrell dust; it refers to the dust particles removed from the gaseous product stream above the furnace by the electrostatic precipitators, which provide the first cleaning stage of the produced phosphorus. Cottrell dust mainly consists of Na₂O, K₂O, ZnO and some F.

- Clay; it is delivered in bulk and stored outside. The largest component of the clay is SiO₂ with an average of 60 - 62 wt%, followed by Al₂O₃ with 20 - 28 wt% and Fe at 2 - 2.5 wt%.

- Water; water residue from the sintering plant and slurry station.
The phosphorus production process description

- Rotschlamm; a filtering residue from the wet acid purification plant.
- STPP; Sodiumtripolyphosphate is a by-product produced by Thermphos International and all residues are recirculated back to the furnaces.
- Dorrschlamm; the residue from the phosphorus filtering process in the furnace plant.

The slurry is added to ensure that the fine phosphate ore brought to the granulators, stick together and form pellets, as well as making sure that the pellets are hard and well bonded after the sintering process. The slurry mixing procedure is a batch process and can follow one of three recipes.

- Recipe A; only recommended when no Cottrell dust is forthcoming from the furnace plant or when the water tank contains too much water.
- Recipe B; when normal diverse quantities are available (Cottrell dust:clay in final slurry mix between 65:35 wt%). In principal the only mixture ever prepared.
- Recipe C; when no water is added to the mix.

Recipe B starts of with the addition of water to the Cottrell dust suspension, with the mixture obtaining a density of between 1100 - 1150kg/m$^3$. STPP is then added in order to improve the suspension ability of the clay particles and is always added before the clay. A minimum of 500kg is recommended and based on average plant values. Half a ton of STPP is added to every 10 tons of clay. It is also at this point that any excess Rotschlamm from the wet acid purification plant is added to the mix, the amount of which may vary. Finally, clay is added to the process. The mixing process is complete when the blend density reaches the desired level (1230kg/m$^3$).

The slurry station has two mixing tanks with individual holding abilities of 40m$^3$ and a single batch will provide the granulators with $\approx$5 hours of slurry. Mixing is achieved through the use of a specialised pump that mixes, pumps and has size-reduction ability all at the same time.

Table 2.4: An average slurry composition

<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crushed phosphate rock</td>
<td>84%</td>
</tr>
<tr>
<td>Water</td>
<td>8%</td>
</tr>
<tr>
<td>Clay</td>
<td>5%</td>
</tr>
<tr>
<td>Rotschlamm</td>
<td>1.5%</td>
</tr>
<tr>
<td>Cottrell dust</td>
<td>1.5%</td>
</tr>
</tbody>
</table>

Currently 7.8 wt% of the material fed to the granulators, are slurry. Trouble-free operation of a phosphorus furnace requires that the solid burden in the furnace has relatively constant gas permeability throughout its volume, a scenario that will become increasingly unfeasible if fine particles (less than 1mm) are fed to the furnace. Upon delivery, the purchased phosphate ore is therefore unsuitable for furnace operation and needs to be pelletised, with the slurry serving as a binder.
2.6.4 Phosphate ore

All the phosphate ore is not necessarily acquired from a single source. Owing to economic factors the phosphate ore storage facility can therefore, at times, be stocked with different types of ore. The two main types of phosphate ore are (1) magmatic ore consisting mainly of fluorapatite, calcite, dolomite and quartz and (2) sedimentary ore consisting mainly of fluorapatite, quartz and sometimes a fraction of calcite. From the storage facility the desired mixture between the magmatic ore and the sedimentary ore is sent to the sinter plant where it is ground in a mill and screened at 250mm. The smaller particles will proceed to an intermediate storage tank, while the bigger particles will re-enter the mill via the return stream or circulating load. The circulating load also consists of disapproved pellets, as well as phosphate and coke dust from the sinter plants. It is from these intermediate storage tanks that the phosphate ore is fed to the disk granulators and pelletised. On average 80 wt% of the material fed to the granulators consist of fresh feed, with the other 20 wt% made up of return load.

2.7 Granulators, pellets and sinter plant

Pellet production is carried out with disk granulators, where pellets are produced with moderately constant slurry-to-phosphate ore ratio of 1:6. The production procedure dictates that 60% of the pellets must be larger than 12.5mm. Sometimes Rotschlamm is also added. When modification to the mixture ratio is required, the slurry flowrate is adjusted manually by the operator based on visual observation, a skill acquired only through a wealth of experience. Roasting of the pellets produced is carried out with Lepol roasters. The moist phosphate pellets pass via the feeder into the drying zone of the roaster where they are dried by the exhaust gases from the combustion zone and by the hot air from the cooling zone at the end of the roaster. The heat for roasting the dried pellets is provided by combustion of phosphorus furnace gas (85-90% CO) in the burners at temperatures exceeding 800°C, in which other fuels such as brown coal dust can also be used if there is insufficient gas. After the roasted pellets have passed through a dwell zone, they pass to the cooling zone where they are cooled by drawing cold air through the bed of pellets. The process makes efficient use of the heat of combustion of the fuel gas. The gases from the sintering process are removed by an extraction fan via a wet scrubber or other gas washing equipment. After a residence time of approximately one hour inside the Lepol roaster, the pellets are once again screened (roughly 10 wt% returned to the mill) to ensure the removal of overly fine particles that can be detrimental to the furnace.

2.8 The submerged arc furnace for phosphorus production

The furnace casing is made of sheet steel, the lower part lined with hard blocks of strongly calcined carbon, and the upper part with firebrick. The floor and lower part
of the furnace are water-cooled. The furnace is shaped like an equilateral triangle with rounded corners. The three electrodes are situated at the corners of a regular triangle. Two of the furnaces are equipped with pre-baked electrodes, while the third furnace is equipped with Söderberg electrodes. The material of the Söderberg electrodes is heated by the electrical current and the furnace heat and is baked solid in the region of the contact plates. The electrode must become baked solid over its entire cross section when it is fed downwards to compensate for its consumption in the furnace (a few centimeters per hour). If the electrodes are not completely baked, there is a risk of breakage, especially with long electrodes. Söderberg electrodes have a higher proportion of organic impurities when compared to the pre-baked electrodes which is the reason why the Söderberg furnace produces yellow phosphorus. The electrode current is kept fairly constant during operation by automatically raising and lowering the electrodes; i.e., if the current increases, the electrodes are raised, increasing the electrical resistance between the electrodes and the furnace floor and hence reducing the current, and vice versa (combined with keeping voltage constant).

Figure 2.3: Top view of the submerged arc furnace.

Another 40% is consumed by the heat content of slag, ferrophosphorus and furnace gases, while the remaining 15% is expended through electrical losses, radiation losses and cooling water losses (Robiette and Allen, 1972). As can be seen from Figure 2.3, there are four feed chutes surrounding each electrode. The middle three combine to form a wider pipe. Since the furnace is operated under slight overpressure, nitrogen is continuously fed into the charging bunker, so that no carbon monoxide can reach the charging platform. These feed chutes extend from the top of the furnace to more
2.9 Gaseous product, liquid phases and downstream equipment

than 20 meters up in the air. Here they are systematically fed through an conveyor belt system that ensures that none of the feed chutes become empty. For the purpose of this report the small parts of the feed chutes that protrude into the furnace will be referred to as the internal feed chutes and the more than 20 meter parts the external feed chutes. The lifetime of a phosphorus furnace is mainly determined by the durability of the carbon lining. Detailed monitoring of the state of the lining does not necessitate shutting down the furnace and completely emptying it. It is achieved by incorporating radioactive sources at points where erosion is known to occur. Special thermocouples are inserted at various depths in the carbon bricks to continuously measure the wall temperature. These temperatures serve as a maintenance tool, alerting the system to any irregularities. It is crucial to monitor the position of the wear line in order to avoid hot metal or slag from breaking through the lining and cause damage to the operators, the furnace and nearby equipment. This type of industrial monitoring is not only important for maintaining high standards of safety but also serves an economic purpose. Although the gaseous product leaving a furnace mostly comprises of P\textsubscript{4} and carbon monoxide it still needs to be purified from any dust and is sent to an electrostatic gas purification system. This and the rest of the downstream products and equipment are discussed in Section 2.9.

2.9 Gaseous product, liquid phases and downstream equipment

2.9.1 Slag

At 550000 tons per year the slag produced at Thermphos International is the product made in the largest quantity. The liquid slag is sequentially tapped from the furnace through two tap holes and stored on a large dump. For each ton of phosphorus, about 7 tons of slag is produced. The smooth tapping off of this slag at between 1350-1450°C determines to a considerable extent the production rate of a furnace. The furnace has two slag tap holes positioned in such a way (located 400mm above the furnace floor) to enable the slag to be tapped symmetrically. The holes are alternated every four hours and must therefore be wear-resistant. There are water-cooled metal devices built into the carbon blocks of the furnace lining and they can be closed with water-cooled metal plugs. The slag, used in the construction of roads, does not only contain the waste material from the process but also some displaced phosphorus. The yield of phosphorus, if only in part, depends on the P\textsubscript{2}O\textsubscript{5}(slag). Not only the analysis of the raw material must be monitored, but continuous analysis of the slag produced is also essential. With good furnace operation, P\textsubscript{2}O\textsubscript{5}(slag) can be held to 1.7 wt%. Since it can carry a small percentage of phosphorus and requires considerable heat to melt, it is important to cut the slag volume to a minimum. Examination of the phase diagram of the CaO-SiO\textsubscript{2} system indicates two eutectic points. This phase diagram is seen in Figure 2.4, where these two points are indicated. The one corresponds to 3CaO.2SiO\textsubscript{2} with SiO\textsubscript{2} at 42 wt% and a melting point of 1460°C. The other point corresponds to CaO.SiO\textsubscript{2} with the slightly lower melting point of 1430°C but with a SiO\textsubscript{2} content of 62 wt%. The negative effects of this increased slag volume at a SiO\textsubscript{2} content of
62 percent, however, far outweighs the potential energy savings brought on by the 30°C decrease in melting temperature of the slag. It is therefore more economic to aim for the first eutectic point (Robiette and Allen, 1972).

Thermphos International defines its basicity ratio as \( \frac{\text{SiO}_2}{\text{CaO}} \) and its value controls the flow properties of the slag. The amount of silica addition is determined with this ratio and in practice a value of between 0.85 and 0.95 is achieved.

**Figure 2.4:** The binary phase diagram of the CaO-SiO\(_2\) system.

### 2.9.2 Ferrophosphorus

The furnace produces ferrophosphorus, which collects under the slag. The ferrophosphorus is tapped off, usually once per day, through a hole in one of the carbon blocks, which is opened with an oxygen lance and closed again with a clay plug. The ferrophosphorus, together with some slag, overflows into a bed of sand. Depending on the method of furnace operation, the ferrophosphorus contains between 15 and 28 wt% P, corresponding approximately to the formula Fe\(_2\)P and FeP. An electron scan image of the two corresponding phases taken at Delft University of Technology can be seen on the left-hand side of Figure 2.5. The more extensively the phosphate rock is reduced, the more silica is converted into silicon, which reduces the phosphorus content of the ferrophosphorus. The
2.9 Gaseous product, liquid phases and downstream equipment

Combined content of P and Si is 25 - 30wt%. Approximately 45% of the Fe fed to the furnace leaves the furnace with the ferrophosphorus and the rest as droplets with the slag.

During another study on the Fe-phosphide phase formed during phosphorus production in a submerged arc furnace conducted in parallel at Delft University of Technology, a sample of ferrophosphorus containing uranium-bearing Fe-phosphide was found. This compound had not been described before and an electron scan image of the phase can be seen on the right-hand side of Figure 2.5. Uranium, as well as other trace metals like Mn, V, Cr, Ni, Zr, originates from the apatite ore used. Ti originates partly from the silica and coke used in the reduction process, but mainly from the clay used to produce ore pellets. Voncken, Scheepers and Yang (2006) described the ferrophosphorus with respect to composition and crystalline compounds present. The crystallization sequence is discussed with respect to the FeP-phase diagram. The main phases found in the ferrophosphorus are FeP and Fe$_2$P. With respect to trace and minor metals, it is observed that Si preferably enters the FeP-phase, whereas Ti, V, Cr, Mn and Ni preferably enter the Fe$_2$P-phase, which is an analogue of the mineral barringerite. This study gives some insight into the behavior of impurities during crystallization of an iron-rich Fe-phosphide melt.

![Figure 2.5: Left: an electron scan image clearly indicates the two phase, FeP and Fe$_2$P in the ferrophosphorus sample. Right: an electron scan image of the uranium-bearing Fe-phosphide phase (Voncken, Scheepers and Yang, 2006).](image)

2.9.3 Phosphorus

The gaseous product leaves the furnace through two symmetrically spaced outlet vents situated above the ferrophosphorus tap hole in the roof of the furnace. The phosphorus is removed from the gas in three stages:

- Stage 1: the electrostatic precipitators for removal of dust.
- Stage 2: the condensation equipment with the receivers for the phosphorus produced.
- Stage 3: the final filtration equipment

Electrostatic gas purification system  Although the gaseous product leaving a furnace mostly comprises out of $P_4$ and carbon monoxide gas, it still contains an unacceptable amount of dust particles. Between 98 - 99% of the dust, also called Cottrell dust, is removed from the gaseous product by passing it through an electrostatic gas purification system, consisting of two electrostatic precipitators (ESP) for each furnace. The dust is separated from the gas and is deposited into slurry tanks situated underneath the precipitators by a raking arm. Cottrell dust mainly consists of $Na_2O$, $K_2O$, $ZnO$, and F. There is also a chance that the Cottrell mixture might contain phosphorus in the form of $P_2O_5$ (white, odourless fumes) or $PH_3$ (colourless, garlic-smelling fumes). To ensure that these toxic and highly explosive gasses do not form, the pH of the slurry must kept at below 7 through the circulation of water. The Cottrell mixture is continuously recirculated, as well as mechanically stirred and when the slurry reaches a density of between 1230-1250kg/m$^3$, it is pump to one of two holding tanks with individual storing capacities of 15m$^3$. Each holding tank can accommodate four slurry tanks. An average of 10000 tons of dust (Cottrell dust) per year is slurried with water and recycled back to the slurry plant where it will be used as a binder for the agglomeration of the phosphate rock on the granulators. The temperature in the precipitator must exceed the boiling point of phosphorus (280°C) in order to prevent premature condensation of the phosphorus. The gaseous product stream temperature, however, is usually high enough to prevent condensation. Care should also be taken not exceed 600°C. Beyond this temperature the efficiency of electrostatic precipitators decreases and the equipment could be damaged.

Dezincing station  Owing to recirculation of Cottrell dust, Zn and certain radioactive material like Pb 210 en Po 210, tend to build up in the process and are systematically removed at the dezincing station. A high pressure filtering technique is employed to rid part of the Cottrell slurry stream of these potentially damaging elements. The filter cake is then heated to purge it of any trace elements of potentially flammable phosphorus, as well as excess $H_2O$. The resulting product is calcinate and is stored in closed containers. These containers are then sent to a specialised company, where they will be stored for a period of 150 years.

Condensation and collection system  The virtually dust-free furnace gases enter the condensation system. There are hot and cold condensation stages. The hot stage operates above the melting point of phosphorus and the cold stage below it. In both cases, the gas is washed with water, causing the phosphorus to condense from the gas stream. The hot condensation equipment consists of two fall-down pipes (800mm in diameter), one washing tower and one hot bottom tank. Sprayers are situated on the inside of the fall-down pipes and the hot condensation tower. Warm water from the hot bottom tank (about 60°C) is circulated through these sprayers, ensuring that more than 97% of the gaseous phosphorus is condensed and fed to the hot bottom tank.
2.10 Automated control of the furnace process

Filtration  The phosphorus must be filtered in order to remove impurities which would affect the quality of the product. These impurities consist mainly of fluorine compounds derived from SiF$_4$. This first forms hexafluorosilicic acid, which then hydrolyzes in the condensation equipment and stabilizes the sludge formed by the dust and phosphorus. Table 2.5 gives an average sludge analysis.

<table>
<thead>
<tr>
<th></th>
<th>Good furnace operation</th>
<th>Unstable furnace operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>P$_4$</td>
<td>30-40wt%</td>
<td>70-80wt%</td>
</tr>
<tr>
<td>Cottrell dust</td>
<td>about 10wt%</td>
<td>about 10wt%</td>
</tr>
<tr>
<td>Water</td>
<td>60-50wt%</td>
<td>20-10wt%</td>
</tr>
</tbody>
</table>

The process produces in excess of 75 - 100kg sludge per ton of P$_4$ produced and is fed to a holding tank (2m$^3$) before being periodically recycled back to the furnace. Put another way, it requires 10MW to produce $\approx$100 liters of sludge (at a density of 1300 - 1400kg/m$^3$).

2.9.4 Additional gas

For every ton of P$_4$, about 2500Nm$^3$ of additional gas (from here on referred to as FOG) is produced, with a further 30 - 40g of Cottrell dust per Nm$^3$. Ninety percent (90%) of the FOG is used as a fuel in the sintering plant, the phosphate salt plant and by the ESP. The other 10wt% is flared off. The FOG is not analysed on a regular basis, but an average analysis is seen in Table 2.6.

<table>
<thead>
<tr>
<th>Composition</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>86wt%</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>2wt%</td>
</tr>
<tr>
<td>H$_2$</td>
<td>3wt%</td>
</tr>
<tr>
<td>N$_2$</td>
<td>7wt%</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>0.8wt%</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>0.6wt%</td>
</tr>
<tr>
<td>H$_2$S</td>
<td>0.1wt%</td>
</tr>
<tr>
<td>HCN</td>
<td>0.15wt%</td>
</tr>
<tr>
<td>HF</td>
<td>0.01wt%</td>
</tr>
<tr>
<td>P</td>
<td>80 ppm</td>
</tr>
<tr>
<td>PH$_3$</td>
<td>500 ppm</td>
</tr>
</tbody>
</table>

2.10  Automated control of the furnace process

The next two section are devoted to some of the control procedures at Thermphos International. There are two main types of control which are automated control and operator control. Before discussing automated control, some basic knowledge of the electrical components of a submerged arc furnace is required.
2.10.1 Electrical components of the furnace

The electric components of a three-phase submerged arc furnace can be divided into the following parts:

- The step-down transformer, with its connecting circuit-breaker
- The secondary busbars connected to the low-voltage side of the transformer
- The flexible cables, which connect the stationary busbars to the electrodes and allow vertical movement of the electrodes
- The electrode column, which consists of bus-tubes linking the cables to the electrode contact pads with their operating mechanism. This column is equipped with an electrode dust shield and means for raising and lowering, as well as slipping the electrodes.
- The electrodes, which deliver the current to the furnace feed material.
- The Moeller feed or charge, which acts as the resistor developing the energy required to promote the chemical reactions.

The charge forms the major resistance of the furnaces’ electrical circuit with the other resistance components; the ohmic resistance of the busbars, flexible cables and the electrodes being negligible in comparison. Before discussing the electrical resistance of the charge (packed bed) and its role in furnace control it is important to cover some basic circuit theory relevant to alternating current (AC) systems.

**Resistance, reactance, impedance and power factor**

The electrical circuit consisting of the components discussed above has a variable resistance in the form of the charge, as well as a constant reactance. Reactance (X) is a form of opposition that electronic components exhibit to the passage of alternating current (AC) because of capacitance or inductance. In some respects, reactance is like an AC counterpart of DC (direct current) resistance. The two phenomena, however, are different in important ways, and they can vary independently of each other. Resistance and reactance combine to form impedance, which is defined in terms of two-dimensional quantities known as complex number, which is beyond the scope of this study. The cosinus of phase angle between the voltage and current (cos $\phi$) is called the power factor. A power factor of one or "unity power factor" is the goal of any electric utility company since if the power factor is less than one, more current has to be supplied for a given amount of power use. In so doing, they incur more line losses. They also must have larger capacity equipment in place than would be otherwise necessary. As a result, an industrial facility could be charged a penalty if its power factor is much less than 1. In the case of Thermphos International, the reactance of the circuit remains constant, resulting in some fluctuations occurring in the power factor. For a DC circuit the power is $P = V \cdot I$ and this relationship is also true for the instantaneous power in an AC circuit. However, the average power in an AC circuit with three electrodes expressed in terms of the voltage and current
is \( P = V \cdot I \cos \phi \cdot \sqrt{3} \). In the furnace, the constant reactance value is governed by the design or configuration of the electrical equipment and is an electrical problem which requires a great deal of experience.

### 2.10.2 The electrical resistance of the Moeller charge as part of the electric circuit

The charge forms the major resistance of the furnaces’ electrical circuit. At the top of this charge (top of the packed bed) in the furnace, where only solid pellets, coke particles and silica pebbles are present, no current flow occurs between the electrodes because of the high electrical resistance of the charge. However, as the raw materials descend towards the reduction zone around the electrode tips which are buried in the charge, the non-carbonaceous part of the charge begins to melt, significantly lowering the electrical resistance. A conductive path is thus provided between the electrodes where the ohmic energy \( (I^2R) \) is released to attain the high temperatures and energy levels necessary to effect the Wöhler reaction of Equation 2.3. The stability of the charge resistance is vitally important to the stable operation of the furnace process. In this regard, the gravitational feed system ensures relative continuity in the smelting process and provides a stable electrical load which can, however, be disturbed by e.g. partially fused material in the upper charge layers forming hard crusts, or bridges which prevent descend of the charge into the reduction zone. This phenomenon is called bridge-forming, where large volumes of hot gases formed in the reduction zone, which normally freely escape through and preheat the overlying solid porous descending charge, are partially trapped below the crust, building up pressure until eventually the hot gas bursts through in a volcanic manner, throwing up molten material and temporarily disturbing the electrical circuit. Apart from these major disturbances, some smaller disturbances can come about through coke segregation, heterogeneous particle size distribution, large temperature differences and the introduction of colder feed. These changes are dependent variables and can not be controlled directly, but can be corrected in a feedback way. This is all brought about through the constant-current control principle adopted at Thermphos International, the concept of which is discussed in Section 2.10.3.

### 2.10.3 The principle of constant-current and it role in furnace control

The energy provided to the furnace through the electrode is electrical power that is converted to heat and for AC electrical power it means that if a voltage \( V \) is applied over a resistance \( R \), a current \( I \) will flow through this resistance. At Thermphos International, the submerged arc furnace electrodes are delta-connected to a common earth, the molten product, with the bulk of the circuit resistance already established as being the charge between the individual electrode tips and the molten product. According to Ohm’s law and assuming a power factor of one, the current is given as \( I = \frac{V}{R} \) with \( P = \frac{V^2}{R} \) obtained from simple substitution. Controlling the power is therefore possible in two ways; by changing the voltage or changing the resistance:
Voltage is regulated on the secondary side of the step-down transformer. For two of the furnaces at Thermphos International the voltage can range from 50V to 700V with steps of 19.1V. Any change in voltage will induce a change in the current of the process. For this reason, during stable operation the voltage value remains constant and can only be changed by the operator if unstable conditions so require.

The main furnace control is focused on keeping the current through the electrodes at a constant value. It is this current that is used to control the energy provided to the furnace through a constant-current control system, for normal operating conditions, the current per electrode ($I_{elec}$) must be maintained at between 58 and 62kA. The current is kept constant by controllers which give a signal to the electrode hoist equipment to lift the electrode whenever any decreases in resistance increases the current. An increase in electrical resistance has the reverse effect in decreasing the current, so that the signal from the controller causes the hoist to lower the electrode to a position where the correct current value is restored. At Thermphos International the constant-current controller measures the individual electrode resistances continuously and corrects the operating height of each electrode every ten seconds. The operating heights of the electrodes are therefore semi-dependent variables with any changes induced as a direct result of operating conditions inside the furnace and current control. All six electrodes on Furnace 1 and 3 have a vertically adjustable range of 1.32m. It is therefore important to note that the operating depth of an electrode as used in this report refers to its position relative to the vertical position in the furnace roof. Both changing the resistance and changing the voltage can therefore be used in controlling the process, but only the resistance is automatically controlled at Thermphos International.

2.11 Feedback operator-induced control of the furnace

The furnace requires knowledgeable operators to assist the automated control system. Where the automated control loops ensure corrections within a couple of minutes, for the Thermphos International process the operator-induced control loop can typically take about 8 hours. In these 8 hours the operators have to optimally steer the process towards a range of setpoints that include $P_2O_5(slag)$. This is facilitated through adjustments to the Moeller feed recipe. The information necessary to calculate these adjustments to the feed recipe is obtained in a feedback way from the chemical analysis performed on the output streams namely slag, gaseous product and ferrophosphorus. Feedback control may be defined as the use of difference signals, determined by comparing the actual values of system variables to their desired values, as a means of controlling a system. An everyday example of a feedback control system is an automobile speed control, which uses the difference between the actual and the desired speed to vary the fuel flow rate. Since the system output is used to regulate its input, such a device is said to be a closed-loop control system. There are also some predetermined settings designed to ensure safe practises. These setpoints, as well as the tools available to the operator in order to induce the
necessary changes are discussed below.

2.11 The ratio of fixed carbon-to-P$_2$O$_5$ addition (C-fix)

In actual operations, fixed carbon control is extremely important. For the addition of coke to the overall Moeller feed, a ratio of fixed carbon-to-P$_2$O$_5$ wt% (C-fix) value is assumed. In general this value is taken as C-fix = 0.465 and called an experience factor. With this value a 5% fixed carbon (C) excess, in relation to the stoichiometric amount of Equation 2.3, is fed to the furnace. This is done for the following reasons:

- To avoid that the carbon lining in the furnace partakes in the reduction process and thereby erodes the furnace
- To compensate for the reduction of impure oxides. The carbon is consumed not only by the reduction of the penta-valent phosphorus in the phosphate, but also in reducing impurities such as oxides of Fe, Ti, Mn and Cr.
- To compensate for the carbon that is tapped with the slag.

This value also takes into account the carbon that is brought into the process by the electrodes. There is, therefore, always a minimum C-fix level below which the process can never be operated, but the possible decrease of the prescribed excess of 5% will be discussed.

2.11.1 The ratio of fixed carbon-to-P$_2$O$_5$ addition (C-fix)

The ratio of coke-to-pellet addition, or coke factor, is almost the same as the C-fix: as long as the P$_2$O$_5$ wt% in the sintered phosphate pellets remain unchanged, the coke factor will have a direct linear relationship to the C-fix. The required quantity of coke to be added to the Moeller is measured out by automatic weighing equipment. Given a standard of 100 tons of sintered phosphate pellet addition, the C-fix = 0.465 can now be used to calculate the necessary amount of coke that needs to be added.

Calculating the coke factor  

P$_2$O$_5$ is added in the form of sintered phosphate pellet and the pellets can have 29 wt% P$_2$O$_5$. Therefore, 100 tons of sintered phosphate pellets contain 29 tons of P$_2$O$_5$. Given a C-fix = 0.465, a total of $(0.465 \times 29) = 13.5$ tons of fixed carbon must be added. This fixed carbon is added in the form of coke (see Table 2.2). This means that $(100:90) \times 13.5 = 15 \left[ \frac{kg \ coke}{100kg \ pellets} \right]$ must be added.

2.11.2 The ratio of coke-to-pellet addition (coke factor)

The amount of silica required for Equation 2.3 is added as silica gravel and is calculated based on what the basicity of the slag should be. Given a standard of 100 tons of sintered phosphate pellet addition, e.g. a basicity $\left( \frac{SiO_2}{CaO} \right) = 0.88$ can be used to
calculate the necessary amount of gravel that needs to be added. The silica gravel factor has units of \( \frac{\text{kg gravel}}{100\text{kg pellets}} \) and is calculated in the following way:

**Calculating the silica gravel factor**  CaO is added with the sintered phosphate pellet and the pellets have 46.9wt% CaO. Therefore, 100 tons of sintered phosphate pellets contain 46.9 tons of CaO. Given a basicity = 0.88, a total of \((0.88 \times 46.9)\) 41.3 tons of silica must be added. The sintered phosphate pellets also contain 13.2wt% SiO\(_2\). This means that 100 tons of pellet bring 13.2 tons of silica with it into the furnace. Along with the coke, 8wt% SiO\(_2\) enters the furnace. With the coke another \((100:8) \times 15\) (coke factor) = 1.28 tons of silica enter the furnace. These amounts should be compensated for, which means that ultimately \((41.3 - 13.2 - 1.28) \times (100:95) = 28.2 \frac{\text{kg gravel}}{100\text{kg pellets}} \) should be added.

### 2.12 Conclusions

The most important driving force of this project was the understanding and minimisation of varying energy consumption created by complex mixtures of primary and as well as secondary, recycled feed materials. In order to achieve this a model is required - a representation of the essential aspects of the process which presents knowledge in usable form. The result was the dynamic model, a CFD model and a dynamic-CFD hybrid model that will be discussed later. With these models the user increases understanding of the sensitivities that exist among the different variables and thus, obtains knowledge on which changes could minimise energy consumption. First and foremost, when constructing such models, in-depth process knowledge is required. This chapter provided a detailed overview of the phosphorus process, as well as introducing such important concepts as residence time of the feed material, reduction zone and the ratio of fixed carbon-to-P\(_2\)O\(_5\) addition (C-fix). These and other concepts or variables will be vital in the construction of the above-mentioned models.

During normal operation the (symmetrically designed, submerged arc) furnace can exhibit some decidedly asymmetrical characteristics. The next chapter will take a closer look at all this asymmetrical behaviour, the causes thereof, if and how these inevitable, asymmetrical manifestations can be minimised and, most importantly, how and to what degree they can assist in the modelling process.
Chapter 3

The symmetrical furnace and its asymmetrical character

Through examination of real industrial data, values from (especially) installed temperature probes in the carbon lining of the furnace and real industrial experiments it was shown that the furnace process exhibited asymmetrical behaviour. To realise this the author spent six uninterrupted months at Thermphos International, entered the empty shells of cold and corroded furnace twice, gathered and analysed more than thirty four mineralogical samples, managed an extensive sampling campaign on the slag stream, performed feed material porosity tests and investigated years of industrial data. These asymmetrical manifestations e.g. unequal distribution of slag tapping time, can be minimised, but at some point no more improvement is possible. For this reason, all the asymmetrical parameters were, in some way or the other, used in the development of the subsequent models. This was done to see if asymmetrical behaviour and especially the recognition thereof, could add predictive ability to models.
3.1 Introduction

Chapter 2 describes in detail the phosphorus producing process as well as the automated and operator control procedures in order to effectively operate the submerged arc furnace. Although these current control practices ensure reliable and safe phosphorus production, the intended control targets e.g. $P_2O_5_{(slag)}$ are sometimes achieved. However, they mostly vary within a wide range of values. This means that any resulting operator-induced control changes are more focussed on correction or damage control rather than on optimisation. This is owing to the extremely distributed nature of process parameters and heterogeniety of the packed bed in the submerged arc furnaces. These parameters include complex burden conductivities, changing mineralogy and liquidus temperatures as functions of changing oxidation states of the constituent minerals, complex flow rates of material affected by smelting ranges under independently operating electrodes and constantly changing temperature profiles in the furnace due to changing arc lengths. All these unpredictable parameters negatively influence control and this is ultimately manifested in asymmetric behaviour of the furnace. The rest of this chapter contains evidence of this in detail.

3.2 The evidence of asymmetrical furnace behaviour

The submerged arc furnace as seen in Figure 1.1 is designed symmetrically. Standard operating procedures also dictate that the furnace should be operated in a symmetrical way e.g. the two slag tap holes should be tapped 50-50%. In practise, however, the furnace displays some decidedly asymmetrical characteristics, the most obvious consequence of this being the excessively lopsided erosion captured by an infrared scanning technique during a full inspection and maintenance shut-down of Furnace 1 during January and February of 2004 (see Figures 3.1 and 3.2). The following sections will look at the individual aspects that highlights the asymmetrical behaviour and the following questions will be answered:

- Which parameter or variable exhibits asymmetrical behaviour?
- Which data were used to identify the asymmetrical behaviour and which data filter was applied?
- What were the causes of the asymmetrical behaviour?
- How can the recognitions of similar symptoms be utilised to optimise current furnace operations?
- What is the potential impact of asymmetrical furnace behaviour on phosphorus recovery?
- Can the recognition of asymmetrical symptoms assist in the modelling process?

Little reference will be made of conditions associated with the middle electrode. This is done because it is situated on the symmetrical plane of the furnace and has
3.2 The evidence of asymmetrical furnace behaviour

3.2.1 Individual electrode resistance and power consumption

**Data and filtering techniques**  The resistances between the individual electrodes and the slag bath showed asymmetrical behaviour. The data range investigated was from March 2000 to December 2003, on Furnace 1 only and 7898 data points (with a frequency of four hours) were utilised.

**Results and discussion**  Table 3.1 represents the average values calculated from unfiltered data. Table 3.2 represents values subject to filtering of one standard deviation. Current and voltage data displayed high degrees of kurtosis (ie. the
The symmetrical furnace and its asymmetrical character

Figure 3.2: The carbon lining erosion found in Furnace 1 during the full maintenance shutdown. The exact location of this erosion is marked in Figure 3.1. The author took this photo.

distribution of the data has a large tail). Owing to the skewness of the data, absolute values between the two tables shows considerably variation. Although filtering had a significant effect on the absolute values, the average disparities between the left and right electrodes remain almost the same at 0.06 mΩ. The power (MW) delivered to the furnace by the individual electrodes showed the same behaviour. The same data and filtering techniques were used for calculating these individual values. The average difference between the left and right electrodes was 0.24MW. With a furnace that has an average overall power consumption of 37MW, that difference represents 0.65% of the total power. A lower mΩ resistance value is the result of higher packed bed conductivity values around the right electrode.

Table 3.1: Average values calculated from unfiltered data

<table>
<thead>
<tr>
<th>Volt</th>
<th>Middle electrode</th>
<th>Right electrode</th>
<th>Diff. between left and right</th>
<th>Diff. between middle and right</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Volt</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>224.2</td>
<td>241.3</td>
<td>220.3</td>
<td>3.9</td>
<td>21</td>
</tr>
<tr>
<td>53.8</td>
<td>54.1</td>
<td>53.6</td>
<td>0.11</td>
<td>0.5</td>
</tr>
<tr>
<td>4.17</td>
<td>4.46</td>
<td>4.11</td>
<td>0.06</td>
<td>0.35</td>
</tr>
<tr>
<td>12.05</td>
<td>13.06</td>
<td>11.82</td>
<td>0.23</td>
<td>1.24</td>
</tr>
</tbody>
</table>

3.2.2 Gaseous outlet temperatures

Data and filtering techniques Data range investigated was from January 2000 to December 2003, from all three furnaces. There were 17531 unfiltered data points with a frequency of two hours. In order to partially compensate for long periods of
3.2 The evidence of asymmetrical furnace behaviour

Table 3.2: Average values of data filtered with one standard deviation.

<table>
<thead>
<tr>
<th></th>
<th>Left electrode</th>
<th>Middle electrode</th>
<th>Right electrode</th>
<th>Diff. between left and right</th>
<th>Diff. between middle and right</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volt</td>
<td>238.6</td>
<td>247.7</td>
<td>234.7</td>
<td>3.9</td>
<td>13</td>
</tr>
<tr>
<td>Current(Amp)</td>
<td>57.9</td>
<td>57.6</td>
<td>57.2</td>
<td>0.06</td>
<td>0.4</td>
</tr>
<tr>
<td>mΩ</td>
<td>4.16</td>
<td>4.3</td>
<td>4.1</td>
<td>0.06</td>
<td>0.2</td>
</tr>
<tr>
<td>MW</td>
<td>13.67</td>
<td>14.27</td>
<td>13.43</td>
<td>0.24</td>
<td>0.84</td>
</tr>
</tbody>
</table>

shut-down and start-up, all outlet temperatures lower than 300°C and higher than 800°C were identified as outliers and filtered from the measured data.

Results  Between 2000 and 2004, substantial temperature differences between the two outlets existed in Furnace 1 and 3. These results can be seen in Table 3.3.

Table 3.3: Temperature of gaseous outlet streams of all three furnaces.

<table>
<thead>
<tr>
<th></th>
<th>A-Left</th>
<th>B-Right</th>
<th>C-Left</th>
<th>D-Right</th>
<th>E-Left</th>
<th>F-Right</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Furnace 1</td>
<td>495</td>
<td>446</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>49</td>
</tr>
<tr>
<td>Furnace 2</td>
<td>-</td>
<td>-</td>
<td>501</td>
<td>499</td>
<td>-</td>
<td>-</td>
<td>2</td>
</tr>
<tr>
<td>Furnace 3</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>543</td>
<td>449</td>
<td>94</td>
</tr>
</tbody>
</table>

3.2.3 Operating height of electrodes

During normal furnace operation the process is current-controlled. As described in Section 2.10.3, when a furnace is running between 30 and 50MW, the controller will attempt to keep the current stable at between 54 and 62A (for Furnace 1 and 3). Any sudden disturbance in individual electrode current is counteracted by moving the electrode up or down in the burden (as well as the other two electrodes according to a preset ratio). The resulting change in resistance stabilises the current. The operating heights of the electrodes are semi-dependent variables with any changes induced as a direct result of operating conditions inside the furnace and current control. By investigating average electrode operating heights, more can be understood about the depth and location of localised resistances and conductivities, the position of the theoretical softening zone, the position of the reaction zone (an extremely important aspect when dealing with the CFD part of this project) as well as finding further evidence supporting other findings mentioned in this document.

Data and filtering techniques  Data range investigated was from January 2000 to December 2003, from only Furnace 1 and 35064 unfiltered data points with a frequency of one hour were utilised. In order to eliminate the incidents when the electrode reached the mechanical limits of the hoist equipment, all data values ≤0.04m and ≥1.31m were filtered.

Results  With no filtering of the data, the left and right electrodes seemed to operated at approximately the same height. Table 3.4 does show, however, that
The symmetrical furnace and its asymmetrical character

the filtered data measures a more significant (relative) operating-height difference between the left and right electrode of 6.1 cm. This difference between the filtered and unfiltered data are owing to the 2001 full hours (see Table 3.5) that the left electrode was operated at its mechanical lower-limit. This typically happens when the current-control system dropped the left electrode in search of lower resistance (higher conductivity) but failed to so. (Furnace 1 data from August 2005 to May 2006 revealed an even more significant operating-height difference between the left and right electrodes of 13 cm). On the other hand, the 14 hours that the right electrode operated at its mechanical lower limits is negligible. That means that optimal conditions was within the mechanical range.

Table 3.4: Average electrode operating heights of the electrodes.

<table>
<thead>
<tr>
<th></th>
<th>Left electrode</th>
<th>Middle electrode</th>
<th>Right electrode</th>
<th>Difference between left and right</th>
</tr>
</thead>
<tbody>
<tr>
<td>No filtering</td>
<td>66.4 cm</td>
<td>73.1 cm</td>
<td>64.6 cm</td>
<td>1.8 cm</td>
</tr>
<tr>
<td>Filtering ≤4cm and ≥131 cm</td>
<td>67.1 cm</td>
<td>71.7 cm</td>
<td>61.0 cm</td>
<td>6.1 cm</td>
</tr>
</tbody>
</table>

Table 3.5: Amount of times individual electrodes operated at a height of ≥131cm or ≤4cm for longer than one hour.

<table>
<thead>
<tr>
<th></th>
<th>Left electrode</th>
<th>Middle electrode</th>
<th>Right electrode</th>
</tr>
</thead>
<tbody>
<tr>
<td>≥1.31m</td>
<td>1639</td>
<td>1723</td>
<td>1767</td>
</tr>
<tr>
<td>&lt;0.04m</td>
<td>2001</td>
<td>780</td>
<td>14</td>
</tr>
</tbody>
</table>

3.2.4 Furnace feed flowrates

Data and filtering techniques Data range investigated was from January to December 2003, from Furnace 1 only and 365 unfiltered data points with a frequency of one day were utilised. No filtering techniques were applied to the data.

Results In Figure 3.3 the average tonnage values of individual feed chutes per day of Furnace 1 during 2003 are shown. The three feed chutes connected exclusively to the left section of Furnace 1 delivered a daily average of 16 tons less Moeller (171 ton/day from feed chute 1, 12 and 11) than the feed chutes supplying the right section of the furnace (187 ton/day from feed chute 7, 8 and 9). The feed chutes in the middle of the furnace (feed chute 2 and 5; number 10 is permanently closed for Furnace 1) provide more than double the average value of the other nine feed chutes. It is however not known to which side of the furnace these feed chutes delivered the feed.

3.2.5 Electrode current disturbances

The aim was to characterise the distribution of electrical current collapses associated with the three electrodes of Furnace 1. In this study, an electrical current disturbance
3.2 The evidence of asymmetrical furnace behaviour

Figure 3.3: Average tonnage values of individual feed chutes per day of Furnace 1 during 2003. Data measured by author and analysed as shown.

is characterised by a decrease of more than 15kA per electrode within the space of one minute and a Moeller burden collapse is a decrease of more than 30kA.

Data and filtering techniques Data range investigated was from 1 to 26 January 2003 and only on Furnace 1. In total 37440 unfiltered data points with a frequency of one minute were utilised. The filter ranges used on the current were 15, 20, 25 and 30kA.

Results Figure 3.4 show that the left electrode consistently had the bulk of the current disturbances and up to 60% of all burden collapses in the furnace.

3.2.6 Slag tapping regime

The aim here was to determine the tapping ratio between the two tap holes of Furnace 1.

Data and filtering techniques Although the data are not directly available, the time spent tapping through individual holes can be calculated by analysing the difference between the inlet and outlet temperature of the cooling water ($\Delta T_{\text{disease}}$) in the cooling system, or disease, around the tap hole (see Figure 3.5).
investigated was from January to May 2003 and only from Furnace 1. In total, 14496 unfiltered data points with a frequency of 15 minutes were utilised. When $\Delta T_{\text{disc}}$ of tap hole A was bigger than tap hole B, tapping at tap hole A was assumed (and visa-a-versa). When both temperature differences registered less than 0.4°C, no tapping was assumed.

**Results** Over the period investigated, 50.7 days was spent tapping through the left (A) slag tap hole, while 73.8 days was spent tapping through the right (B) tap hole. That meant that $\approx 60\%$ of all tapping was done through the right (B) tap hole.
3.2 The evidence of asymmetrical furnace behaviour

3.2.7 Temperature profile of the furnace lining

As standard practice the coke lining of Furnace 1 has six temperature probes embedded at various depths around the slag tap holes. During the full maintenance shutdown of January and February 2004, 8 additional temperature probes were installed in a symmetrical way in the new coke lining of Furnace 1.

![Temperature profile diagram](image)

**Figure 3.6:** Position of additional temperature probes installed in the carbon lining of Furnace 1, as well as their average temperature values between 1 September to 30 October 2004. These data and the statistics of the data will be used to calibrate the CFD model.

In a furnace, where the *inside* is still ill-defined, additional temperature information brings better understanding of the process, which in turn could identify various money-saving alternatives. Apart from the obvious research benefits, additional temperature probes will improve monitoring of the furnace wear line, thus enhancing general safety standards. One crucial aspect in the placement of these probes was the height inside the carbon lining. In order to be utilised efficiently, the probes were placed at a height corresponding to the reduction zone. Another important factor was that they all be placed at roughly the same depth in order to ensure comparability. Another 6 temperature probes were installed vertically, thereby providing information about the temperature profile within the packed bed. Figure 3.6 depicts the positions of these additional temperature sensors that were installed. The values depict the average temperatures of these probes from 1 September to 30 October 2004.
Results  The average temperatures (and corresponding standard deviation) values in Figure 3.6 also emphasize the asymmetrical nature of the furnace if considered that all thermocouples on a horizontal plane were installed at a depth of 0.3 meters. The temperature vary from as high as 384°C to as low as 48°C.

3.2.8 Mineralogy of furnace lining

Data  The full inspection and maintenance shut-down performed on Furnace 3 during January and February of 2005 provided the opportunity to take mineralogical samples from the inside lining of the furnace after removal of the loose material. This took place on 23 to 25 February 2005 when a total of 35 strategic samples were gathered for analysis. Figure 3.7 provides a summary of those analyses and another clear indication of asymmetrical operation.

![Mineralogy of the furnace as sampled by the author and determined by analysis of 35 furnace samples.](image)

3.3 The causes of asymmetrical furnace operation

Varying electrode resistances  When considering that the right electrodes operated at a lower height than the left electrode (see Section 3.2.3) the higher conductivity, as evident in the vicinity of the right electrode, can be brought about by a variety of factors:
3.3 The causes of asymmetrical furnace operation

- The lower height allowed the right electrode to operate closer to the softening and/or liquidus (slag) zone, thus resulting in the higher conductivity. There is, however, no distinct separation of slag and Moeller but rather a mixed zone of semi-reduced, sintered pellets, trapped slag and gaseous product.

- Less negative current fluctuations associated with the right electrode. Large and frequent negative current disturbances at the left electrode of Furnace 1 during January - February 2003 could be attributed to an increase in local resistance. This may be explained by a combination of bridge forming and subsequent collapse of feed around the electrodes that creates instabilities in the current flow. On the other hand, increased throughput of Moeller feed to the three feed chutes associated with the right section of the Furnace 1 might have induced a series of miniature collapses rather than more substantial collapses. A more stable current, as well as a higher, average local conductivity, could be the consequence.

- A higher coke content in the Moeller feed surrounding the right electrode. Rough pilot scale testing done at Thermphos International showed a marked degree of segregate between pellets, coke and silica gravel when allowed to fall fixed distances to the ground. Substantial Moeller collapses in the furnace bed could therefore induce coke segregation, causing changes in conductivity.

Varying gaseous outlet temperatures  Table 3.3 show average gaseous outlet temperatures Temp A (left) = 495°C and Temp B (Right) = 446°C of Furnace 1. A reason for the difference can be found in the substantial difference in Moeller throughput [ton/day] to the right section of the furnace:

- An average of 187ton/day was fed to the right section of Furnace 1. This is the sum of feed chutes 7, 8 and 9
- An average of 171ton/day were fed to the left section of the furnace. This is the sum of feed chutes 1, 11 and 12.

The larger the quantity of fresh (and therefore colder) Moeller that is fed to the right section of the furnace, the more prevalent the heat transfer or exchange will be. The heat exchange takes place in the packed bed. As the gaseous product is produced in the reduction zone, it rises through the unreduced Moeller bed towards the outlet and heat is exchanged between the gas and fresh feed.

Varying furnace feed flowrates

- In the first part of 2003, 60% of all slag tapping was done on the right tap hole with the choice of tap hole up to the operator. This might explain why the right side of the furnace should consumed more Moeller feed.
- Higher average conductivities around the right electrode cause elevated temperatures, which in turn causes the new feed to melt more rapidly.
Varying electrode operating heights For a total of 2001 hours, the optimal operating conditions around the left electrode were located too low in the bed for the mechanical hoist of the electrode to properly respond i.e. it reached its limit. This phenomena happened only 14 times with the right electrode. This showed that optimal operating conditions (as imposed by current set-points) were within the movable range of the right electrode. This would therefore imply that the mechanical hoist restrictions imposed on this dependent variable may be one of the causes why the process deviates. It raises the interesting question of how much the process will benefit from increasing the lower and upper set points for the movement of the electrodes. The amount of times that all three electrodes operated at maximum height is easily explained by the circa 6 - 10 m$^3$ liquid slag/hour that builds up inside the furnace every time the tap holes are closed in order to change full ladle.

Varying electrode current disturbances The filtered data revealed a higher, average operating height for the left electrode. Yet, as already seen from unfiltered data in Table 3.5, it is almost exclusively the left electrode that spent a significant amount of operation time at its mechanical lower limit. These apparent contradictions alone point to fluctuating operating heights for the left electrode. It also implies that the optimal electrode position as dictated by the current set-point, was often located lower than the electrode could reach. Once the electrode can not move any lower in search of lower resistance, it would then be operating at a higher resistance than required causing increased MW values. This results in higher localised temperatures around the electrode - favourable conditions for sintering and bridge-formation. Once a formed bridge collapses, cold Moeller will surround the electrode, causing the resistance around the electrode to increase and cause the sudden change in the electrode current. This raises another interesting question of how much the process will benefit from electrodes that can vibrate. This will enduce a series of controllable mini collapses underneath the electrodes and, hopefully, a more stable process.

Unequal slag tapping It is believed that the, now familiar, asymmetrical behaviour indicated in Figure 3.1 and confirmed by data, largely stems from unequal tapping - the temptation to abandon standard protocol and keep on tapping at the same slag tap hole as long as the slag flows freely. This practise should, however, be weighed against the possible disadvantages of strict enforcement of a 50/50 slag tapping policy on an already eroded furnace. The extensive erosion on the right side of the furnace (Figure 3.2), the slag tapping ratio, the lower operating height of the right electrode (Table 3.4) and the higher Moeller feedrate to the right section of the furnace all describe a furnace with an operational pull towards the right slag tap hole (tap hole B). The lack of current disturbances and the all but negligible 14 hours (compared to 2001 hours) that the right electrode spent at its lower limit point towards an electrode that had the optimum operating conditions within its mechanical hoist range and that had been operationally stable. The opposite conditions endured bridge-formation and burden collapses around the left electrode, making the slag difficult to tap and the tap hole difficult to open. Forcing
3.4 The impact of asymmetrical behaviour on phosphorus recovery

Owing to the large production volume of slag, a seemingly small amount of \( P_2O_5(slag) \) can result in substantial losses of unreduced, potential product. For this reason, the \( P_2O_5(slag) \) values of the two slag streams were compared in order to investigate the reductive conditions around the electrodes and to comment on the impact of asymmetrical conditions on the loss of unreduced product.

**Data and filtering techniques**  The \( P_2O_5(slag) \) values of individual tapping sides are not directly available. To obtain these values, the timestamps associated with each \( P_2O_5(slag) \) value were compared with the slag tapping data from Section 3.2.6. In this way, the \( P_2O_5(slag) \) values of the separate slag streams were determined. The data range investigated was from January to May 2003. The following filtering criteria were applied (see Figure 3.8).

- **Case 1**: Attributing all the Fe in the slag analysis to pure Fe\(_2\)O\(_3\), with no droplets of Fe\(_2\)P entrapped in the slag
- **Case 2**: Attributing all the Fe in the slag analysis to be trapped droplets of Fe\(_2\)P, the \( P_2O_5(slag) \) values were subsequently adjusted to account for the loss of P through droplet formation

**Results**  All results revealed the slag tapped from the left tap hole to have a lower \( P_2O_5(slag) \). This showed that conditions on the left side of the furnace were more effective in reducing \( P_2O_5(slag) \) from the raw material. A lower average Moeller flowrate to the left side of the furnace, however, means a longer residence time in the furnace, thereby providing more time for gas/solid interaction. This result provide more evidence that liberation of the phosphorus from the ore (where most of the \( P_xO_y \) is considered to be \( P_2O_5 \), or gas-solid reduction, is the rate limiting step. This in turn, also indicates that, kinetically as well as thermodynamically, the liquid slag phase voluminously more evident on the right side of the furnace, or gas-liquid reduction, does not represent an optimum reductive environment.

The left electrode had an higher average mΩ value, possibly resulting in higher burden temperatures around the electrode as conduction of electricity through the coke generated more heat (a theory perhaps validated by the 49°C higher average gaseous product outlet temperature on the left of the furnace). \( P_xO_y \) is liberated and diffuses through the pellet to react with C on the surface of the coke. Thermodynamically, the formation of \( P_2(g) \) is enhanced at elevated temperatures. It was thought that extremely high \( P_2O_5 \) wt% values measured (and filtered out) in the slag could be correlated with Moeller collapses underneath the appropriate electrode causing large amounts of unreduced \( P_2O_5 \) to exit with the slag but no correlation was found.
3.5 The standard deviation in the $\text{P}_2\text{O}_5(\text{slag})$ composition

The reduction of variance around a required setpoint is one of the major objectives of process control. The $\text{P}_2\text{O}_5(\text{slag})$ is one of these setpoints around which the furnace is steered. During normal operating practice, the slag is sampled every two hours but not each sample is analysed. Four samples collected over an eight-hour period are submitted for analyses as one combined, crushed sample. The slag sample is analysed using X-ray fluorescence spectrometry (XRF) and can be considered extremely accurate. Therefore, it is important to determine if significant standard deviation exists with regard to the $\text{P}_2\text{O}_5(\text{slag})$ in a single slag sample. To investigate this, a designated sampling campaign was performed.

From the slag streams, 25 equispaced (2 hours) samples were take from Furnace 1. The samples were analysed separately and not combined into collective samples. Together they represented 7 actual Thermphos International samples. These 2-hourly samples were all handled identically, with regard to quenching and assaying of the samples and all sample were similar in size. Table 3.6 shows the results of the analyses. The results show that there exists a 16% standard deviation in the $\text{P}_2\text{O}_5(\text{slag})$.

3.6 Conclusions

All the variables mentioned below were, in some way or the other, used in the development of the dynamic and CFD models discussed later in this study. This
3.6 Conclusions

Table 3.6: The standard deviation of the $P_2O_5$ within individual Thermphos International slag samples.

<table>
<thead>
<tr>
<th>Sample results</th>
<th>Slag 1</th>
<th>Slag 2</th>
<th>Slag 3</th>
<th>Slag 4</th>
<th>Slag 5</th>
<th>Slag 6</th>
<th>Slag 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Average sample results</td>
<td>2.81</td>
<td>2.55</td>
<td>2.97</td>
<td>2.45</td>
<td>3.35</td>
<td>2.58</td>
<td></td>
</tr>
<tr>
<td>Average sample results</td>
<td>1.92</td>
<td>1.95</td>
<td>3.15</td>
<td>1.99</td>
<td>2.85</td>
<td>2.62</td>
<td></td>
</tr>
<tr>
<td>Average sample results</td>
<td>2.70</td>
<td>2.25</td>
<td>2.33</td>
<td>2.48</td>
<td>3.4</td>
<td>2.29</td>
<td>2.14</td>
</tr>
<tr>
<td>Average sample results</td>
<td>2.09</td>
<td>2.24</td>
<td>2.89</td>
<td>2.64</td>
<td>2.93</td>
<td>2.26</td>
<td></td>
</tr>
<tr>
<td>Average standard deviation</td>
<td>18%</td>
<td>16%</td>
<td>16%</td>
<td>11%</td>
<td>23%</td>
<td>19%</td>
<td>11%</td>
</tr>
</tbody>
</table>

was done to see if asymmetrical behaviour and especially the recognition thereof, could add predictive ability to the model. More elaborate discussions follow in Chapters 7 and 9.

Electrode resistances

The individual resistance values were utilised in the development of a linear, dynamic process model. It was found that the individual electrode resistance variables were responsible for a negligible predictive improvement to the model.

Gaseous outlet temperatures

Individual gaseous outlet temperature variables were utilised in the development of a linear, dynamic model. It was found these past values (with a sampling interval of 8 hours) provided little or no predictive improvement to the dynamic model. However, the temperatures of the gaseous product gas in the CFD model are completely dependent variables. This allowed the actual variables to be valuable validation tools in the development phase of the CFD model.

Electrode operating heights

Individual operating heights were utilised in the development of a linear, dynamic model. It was found that these past values (with a sampling interval of 8 hours) provided significant enough influence to warrant its inclusion in model development and also played an integral part in designing the various CFD model scenarios.

Slag temperatures

Slag temperature is not measured online, but a pyrometer is used to measure the temperature daily at a specific time. Analogous data representing the slag temperature were obtained by correlating this pyrometer temperature with the $\Delta T_{\text{disE}}$ at the same time. Data range investigated was from January to May 2003, only Furnace 1 and no filtering techniques were applied. Figure 3.9 shows the difference in $\Delta T_{\text{disE}}$ over a period of about 3 days.
Figure 3.9: The difference in cooling water temperatures for the two slag streams as measured by the author.

Figure 3.10: Correlation between the pyrometer and cooling water temperatures as measured by the author.
Figure 3.10 depicts the standardised values. The slag temperatures are not directly measured but a solid correlation value of 0.59 made it possible to include $\Delta T_{\text{dise}}$ as a variable in the development phase of the dynamic model. However, these past values (with a sampling interval of 8 hours) provided little or no predictive improvement to the dynamic model. The pyrometer temperatures, however, were valuable validation tools in the development phase of the CFD model.

**Additional temperature probes**

The additional temperature probe temperatures were used in the development of the dynamic model. It was found, however, that these variables provided small predictive improvements. The reason for this is the highly dynamic nature of the electrode resistances; the time lag between the arc zone and the temperature probes as a result of the furnace lining, make these values less valuable as variables in a model. These temperatures do, however, become invaluable in the validation phase of the CFD model development.
The symmetrical furnace and its asymmetrical character
Part II

The CONCEPTUAL FRAMEWORK of a DYNAMIC-CFD HYBRID MODEL
Chapter 4

The conceptual framework of a dynamic-CFD hybrid model

4.1 Introduction

A phosphorus producing, submerged arc furnace is continuously fluctuating between the dynamic-driven state and the thermodynamic-driven (see Chapter 4). One single modelling approach will, therefore, never be sufficient and it becomes increasingly difficult for standard thermodynamic and kinetic modelling (as well as the associated software) to provide adequate support for any predictive dynamic model (Reuter and Yang, 2005). A combination of modelling techniques is required. It is for this reason that Scheepers, Yang, Reuter and Adema (2006) proposed a Dynamic-CFD hybrid model, an architecture that employs more than one modelling technique. In this thesis these aspects are integrated from data measurements, data driven modelling and finally CFD.

4.2 The model structure

This proposed model employs continuously updated electrical data in order to optimise the model’s predictive ability, with zero-order hold elements enforced on flowrate and composition data until these variables are resampled. The total concept is expressed mathematically in Equation 4.1 and is modelled on the ARX-type, linear transfer function structure (see Appendix C).

\[
y(t+1) = y(t) + \sum_{i=1}^{f} F_i \cdot x_i(t)_{\text{FLOW}} + \sum_{i=1}^{c} C_i \cdot x_i(t)_{\text{COMP}} + \sum_{i=1}^{e} E_i \cdot x_i(t)_{\text{ELEC}} + Datafile Q \left[ \sum_{i=1}^{d} D_i \cdot x_i(t)_{\text{Derived-CFD}} \right]
\]  

(4.1)

The term on the left side, \(y(t+1)\), represents the predicted \(P_2O_5\) wt% value in the slag for the next timestep. The \(y(t)\) term pertains to the \(P_2O_5\) wt% in the slag.
Figure 4.1: Diagram depicting the proposed architecture of the Dynamic-CFD hybrid model within a predictive control system. Clearly indicated is the vectorised look-up table that provides Derived-CFD variables to the Dynamic-CFD hybrid model. The integration of these aspects in the manner shown in this thesis is one of the contributions of this work.

\[(\text{P}_2\text{O}_5\text{[slag]})\text{ at the current timestep.} \]

The terms \(x_{i(t)}\text{FLOW}, x_{i(t)}\text{COMP}\) and \(x_{i(t)}\text{ELEC}\) refer to flowrate, composition and electrical input variables associated with current timestep, while \(F_i, C_i\) and \(E_i\) refer to the respective parameters associated with the variables. The letters \(f, c\) and \(e\) refer to the respective number of variables.

The Derived-CFD variables are represented by the term

\[\sum_{\text{Datafile } 1}^{\text{Datafile } Q} \left[ \sum_{i=1}^{d} D_i \cdot x_{i(t)}\text{Derived-CFD} \right]\]

and are all generated through the offline use of the three-dimensional CFD model in Part IV. These derived variables represent flowrate, temperature and process data not measurable through routine procedures at Thermphos International and can be loosely compared with the
variables used in state space models (Ljung, 1994) (Kanjilal, 1995). These variables are generated in Part IV and include:

- Pressure drop inside the packed bed \((x_{\text{PressDrop}(t)\text{Derived-CFD}})\) (e.g. 45 Pa in Figure 9.19)
- Gaseous product mass flowrate in the outlet ducts \((x_{\text{GasFlow}(t)\text{Derived-CFD}})\) (e.g. 1.63 \(\text{kg/s}\) in Figure 9.20)
- Gaseous product temperature in the outlet ducts \((x_{\text{GasTemp}(t)\text{Derived-CFD}})\) (e.g. 832K in Figure 9.17)
- Specific power consumption (SPC) of the process \((x_{\text{PF}(t)\text{Derived-CFD}})\)
- Volume and shape of the reaction zone inside the packed bed \((x_{\text{VolRedZone}(t)\text{Derived-CFD}})\)
- Strategic temperature gradient values inside the packed bed \((x_{\text{TempGrad1}(t)\text{Derived-CFD}})\) (see Figure 9.18)

Upon solution of every individual offline model, the above-mentioned variables are transferred to an accessible, easy-to-use datafile. Each solved model (and therefore each corresponding datafile) becomes a function of a specific set of input parameters. Over a wide range of varying input variables and boundary conditions, the CFD model is solved for \(Q\) amount of cases, with each solution representing a different scenario (and therefore datafile). All these various datafiles are stored within a database and these variables are referred to as the Derived-CFD variables. The term \(D\) refers to the parameters associated with each of the Derived-CFD variables and \(d\) refers to the amount of Derived-CFD variables in the datafile.

4.3 The link between Dynamic and CFD data

It is now theoretically possible for the ARX-type model, at every timestep, to evaluate its own set of input variables, automatically access the above-mentioned database, identify the CFD datafile that matches its own input conditions, extract the derived variables contained within the datafile, utilise them in the same way as any other regular measured variable as seen in Equation 4.1 and predict one timestep in the future.

After defining the model structure, the question arises how this dynamic-CFD hybrid model could be used to control the furnaces or, alternatively, to suggest good setpoints for operation. Development procedures for such controllers are beyond the scope of the study, but a brief introduction will be given here as to how control may be implemented. In this way the reader is already shown the next step in optimising plant control after obtaining a model.
4.4 Model predictive control

Once a reliable predictive control model like the dynamic-CFD hybrid model has been developed, it can be incorporated into a model predictive control architecture. Model Predictive Control (MPC) is an advanced method of process control that has been in use in the process industries since the 1980s and has a generalised approach to multiple-input multiple-output (MIMO) control, where the process model is used to predict future outputs (Reuter et al., 1996).

Model predictive control is defined as a control scheme in which the controller repeatedly determines or optimises the manipulated variable profile, that optimises an open loop performance on a time interval extending from the current time plus a prediction horizon. Feedback is incorporated by using process measurements, as soon as they become available, to update the optimisation problem for the next time step. Such a control system does not have to be the primary controller but could provide decision support to operators on top of an already-existing control structure. Figure 4.1 shows the graphical representation of the proposed Dynamic-CFD hybrid control model and how it could be implemented to provide decision support.

4.5 Outline of the rest of the study

The rest of the book explains the step-by-step construction of this Dynamic-CFD hybrid model:

- Part III starts by examining the dynamic part. This involves the investigation of industrial data and the reconciliation thereof. It presents details of all experiments performed at the laboratory, as well as on site. It then uses all the obtained information to evaluate and compare the appropriateness of both linear and non-linear modelling techniques. From this, a suitable dynamic linear model structure is chosen with which to proceed.

- Part IV first elaborates on some fundamental theory before proceeding with the construction of a CFD model. All the information contained in the preceding chapters is integral in its successful development: (i) It draws on the reconciled data to build authentic input data, as well as initial- and boundary conditions. (ii) It utilise in-depth process knowledge (from Part I) and furnace dimensions to produce an accurate virtual copy of the submerged arc furnace with real material properties. (iii) Then, together with the above-mentioned data, kinetic- and thermodynamic information are also used to create two sub-models that form the heart of the CFD model. (iv) Finally, experimental and industrial data are used to validate modelling results.
Part III

The DYNAMIC MODEL
Chapter 5

Industrial data investigation, data reconciliation and soft-sensoring

A data mining exercise shows that the common practice of compensating for increased P$_2$O$_5$ in the slag by increasing the fixed carbon-to-P$_2$O$_5$ ratio in the packed bed, has limited effects over the long term. P$_2$O$_5$ in the slag was largely independent of the fixed carbon-to-P$_2$O$_5$ ratio and mostly a function of furnace residence time. At an operating range of higher than average Moeller flowrates combined with lower than average fixed carbon-to-P$_2$O$_5$ ratios, the specific power consumption [MWh/ton P$_4$], is at a minimum but P$_4$ recovery from the Moeller is also at a minimum. In addition a cost analysis exercise reveals that a control strategy that favours a drive towards lower SPC and not higher P$_4$ recovery (less P$_2$O$_5$(slag)) will result in higher profits.
5.1 Introduction

Chapters 2 described the theoretical and chapter 3 the practical day-to-day aspects of a submerged arc furnace and asked if a qualitative understanding of the asymmetrical deviations can improve a model’s predictive ability? Chapter 4 presented a conceptual framework of a model called a dynamic-CFD hybrid model. The first step towards the development of this (and any) model is a thorough investigation of the process data. Such an exercise starts by reconciling the data within their inherent variance in order to close mass balances and estimate some important variables that is not measured online like the flowrate of slag at Thermphos International. It also reveals the most influential process variables, as well as showing how and by how much variables like C-fix and $\tau_{tot}$ influence each other. This chapter takes a look at the data mining exercise performed on Thermphos International data. Finally, a furnace operating cost analysis exercise will reveal the focus areas for optimal furnace production.

5.2 Raw industrial data investigation in view of developing a dynamic model

Different approaches can be used to investigate industrial data. It was decided early on to quantify the operating sensitivity of the furnace variables over C-fix and residence time ($\tau_{tot}$) ranges, as well as the influence their variation has on the $P_2O_5$ loss and the specific power consumption (SPC). C-fix represents an important independent variable, $\tau_{tot}$ is the most influential dependent variable, while $P_2O_5^{(slag)}$ and SPC represent the best measure of a successful process.

Industrial data ranging from January 2003 to September 2006 were divided into 5 groups of decreasing Moeller flowrate ranges (see Figure 5.1). Each individual flowrate group were arranged with descending C-fix values, allowing other variables to be investigated over this operational range representing all probable conditions at Thermphos International.

5.2.1 The relationship between residence time and Moeller flowrate

Unless mentioned otherwise in this report, the furnace residence time ($\tau_{furnace}$) has a direct relationship with the Moeller flowrate and is mathematically expressed in Equation 5.1.

$$\tau_{furnace} = V_{pb} \cdot fr \cdot \rho_{pb} \cdot (1 - \phi_{pb}) \cdot m_{Moeller} \quad (5.1)$$

In Equation 5.1, $V_{pb}$ is the volume of the packed bed in the furnace, $fr$ is the fraction of available furnace volume occupied by freezeling, $\rho_{pb}$ is the bulk density of the packed bed, $\phi_{pb}$ is the void fraction of the packed bed (porosity) and $m_{Moeller}$ is the flowrate of the Moeller feed material through the furnace. To obtain this relationship it was assumed that the packed bed porosity and heap density remain constant, the
5.2 Raw industrial data investigation

Figure 5.1: The data ranges used to evaluate important variables over an operational range.

packed bed has a constant volume and that the flow of the charge through the furnace is plug flow. The heap density of the Moeller before the onset of melting phase formation was experimentally determined to be 37.7% and the average density of the packed bed was assumed constant at 1843 kg/m$^3$. The freezelining is assumed to be at a constant 5% of the total volume and the gravitational feed system ensures that the packed bed has a constant volume. Therefore, the residence time has a linear relationship with the Moeller flowrate. The corresponding values are listed in Table 5.1.

Table 5.1: The relation between Moeller flowrate and residence time

<table>
<thead>
<tr>
<th>$\tau_{\text{furnace}}$ [hours]</th>
<th>Moeller flowrate [ton/hour]</th>
<th>$\tau_{\text{tot}}$ [hours]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>51.1</td>
<td>8</td>
</tr>
<tr>
<td>6</td>
<td>42.6</td>
<td>9</td>
</tr>
<tr>
<td>7</td>
<td>36.5</td>
<td>10</td>
</tr>
<tr>
<td>8</td>
<td>31.9</td>
<td>11</td>
</tr>
<tr>
<td>9</td>
<td>28.4</td>
<td>12</td>
</tr>
<tr>
<td>10</td>
<td>25.6</td>
<td>13</td>
</tr>
</tbody>
</table>

5.2.2 Phosphorus losses in the slag

A common practice in the phosphorus industry is to compensate for increased P$_2$O$_5$ (slag) by increasing the C-fix in the packed bed, with the desired result a lower P$_2$O$_5$ (slag) through additional reductive power available as a result of the additional coke. Figure 5.2 depicts $P_{\text{slag}}$ (P$_2$O$_5$ (slag) × $\left(\frac{62}{182}\right)$) given the range of conditions specified in Figure 5.1. It shows that this, to a large extent, did not have the
Figure 5.2: $P_{\text{slag}}$ over the operating ranges described in Figure 5.1.

Figure 5.3: $P_{\text{slag}}$ from thermodynamic data (Factsage 5.4.1, 2006)

desired effect; at constant Moeller flowrates, $P_{2\text{O}_5(\text{slag})}$ values were largely independent of C-fix and mostly a function of Moeller flowrate in the furnace. This phenomenon is striking considering all the increases made to the C-fix value in order to decrease $P_{2\text{O}_5(\text{slag})}$ and is contrary to common perception. Thermodynamic calculations (Factsage 5.4.1, 2006) showed that a C-fix $= 0.41$ is still thermodynam-
ically capable of reducing all the $P_2O_5$ present in the Moeller feed (see Figure 5.3). Add to that the additional 5% for safety reasons and a C-fix of 0.43 could already be high enough in order to reduce the phosphorus and ensure safe practices.

### 5.2.3 Phosphorus recovery

Figure 5.4 depicts the recovery of the phosphorus from the original apatite source. A direct relationship between a decrease in $P_{\text{slag}}$ and an increase in recovery is clearly seen, thereby linking these two phenomena. A lower Moeller flowrate (higher residence time) will therefore ensure greater recovery of the product. Reasons for the loss of $P$ at higher Moeller flowrates are:

- Lower $m_{\text{Moeller}}$ means longer residence time in the furnace, thereby providing more time for gas/solid interaction.
- Higher $m_{\text{Moeller}}$ means less time for the reaction to strive towards thermodynamic equilibrium results in higher phosphorus losses.
- Faster moving bed increases changes of cold feed columns to be channeled at the edge of the furnace, thus reaching the slag phase at the side of the furnace.

A complete picture of optimum production conditions (and therefore optimum profitability) is only possible when comparing the two above-mentioned phenomena with production rate of phosphorus $\left[\frac{\text{ton} P_4}{\text{hour}}\right]$ as well as the specific power consumption (SPC) $\left[\frac{\text{MWh}}{\text{ton} P_4}\right]$.
5.2.4 Phosphorus production rate

Figure 5.5 shows the increase in phosphorus production rate ($m_{P4}$) with an increase in Moeller flowrate. This result is to be expected, but is described here owing to its significance in the profitability calculations of Section 5.4.

![Figure 5.5](image)

**Figure 5.5:** Phosphorus production rate over the operating ranges described in Figure 5.1.

5.2.5 Specific power consumption (SPC)

Figure 5.6 shows the combined SPC for all three furnaces. The SPC is the most symptomatic indication of the success of the process and in the area where Moeller flowrates are $\geq$ 25-30 AND C-fix $\leq$ 0.475, the SPC is at a minimum. However, at Moeller flowrates $\leq$ 25-30 (average = 36) AND C-fix values $\geq$ 0.475 the SPC systematically rise with increased C-fix. The possible reasons for this can be:

- Increased conductivity of the overall Moeller bed when the C-fix is increased. This would cause the resistance underneath and around the electrode to drop, automated constant-current control would then force the electrode to counteract by moving up in search of higher resistance. The reaction zone will now establish itself in a somewhat colder and higher area of the packed bed, increasing the SPC.

- Assuming that the overall mass flowrate of the Moeller stays constant, a proportional increase in the cokes in the packed bed will require more energy to heat up to the same temperature.
5.2 Raw industrial data investigation

Figure 5.6: The combined specific power consumption for all three furnaces. Around the indicated area where Moeller flowrates are \( \geq 25-30 \) AND C-fix \( \leq 0.475 \), the SPC is at a minimum.

5.2.6 Furnace operating range of maximum profitability

While the SPC and the P\(_4\) production rate graphs show the same operating zone (Moeller flowrates \( \geq 25-30 \) [ton/hour] AND C-fix \( \leq 0.475 \)) of optimum operation (maximum profitability), the P\(_4\)-recovery and P\(_{\text{slag}}\) graphs report maximum P\(_4\) losses (minimum profitability) around the same area. Therefore, to understand which of these phenomena has the biggest influence on profitability, trends must be investigated as part of a cost analysis exercise.

Cost analysis Cost analysis (or otherwise known as cost accounting) is the process of tracking, recording and analysing costs associated with the furnace operation (The Data Management Association, 2007). Cost analysis can be used to support decision making to reduce the operating costs of a furnace and improve its profitability. However, owing to the fact that the slag-, ferrophosphorus- and P\(_4\) flowrates are not directly measured at each individual furnace and that they are integral to any cost analysis exercise, a data reconciliation was performed around one of the furnaces over a six month period in order to obtain these flowrates in a real-time way. Therefore, it is required to discuss the data reconciliation exercise before the cost analysis study in Section 5.11. Data reconciliation of raw industrial data are also the first step towards the development predictive, dynamic model and will be discussed in detail in Section 5.3.
5.3 Data reconciliation

Often a mass balance based on measured data is not closed. The usual reason is inaccuracy of the measurements as a result of the sampling, measurement and analysis errors. Data reconciliation is a technique that adjusts the raw process data such as flow rate and chemical composition values in order to reduce and possibly eliminate discrepancies in the mass balance. The adjusted data will give a more consistent representation of the actual process. In the process it checks and validates all flow rates and analyses in order to highlight gross errors e.g. on the P-mass balance. The variation of the data values is not performed randomly but is subject to the error margins or standard deviations in the measurements (an example of this is the 16% standard deviation of the \( P_2O_5 \text{ (slag)} \) value in the slag samples discussed in Section 3.5). These error margins or standard deviations are accredited to the various total streams flowing in and out of the furnace as well as to the analyses of each element in each of the respective streams. (A small error margin implies that the measurement or analysis affecting that specific parameter is likely to be more accurate than those for parameters with a large error margin). A significant degree of uncertainty can be associated with industrial data and it makes no sense to develop a model - which supposedly predicts process behaviour to a higher accuracy than the inherent total variance associated with a variable. Therefore, a first step towards the development of a predictive, dynamic model is to reconcile the data within their inherent variance. The experience of the plant personnel is incorporated in the calculation, as is measurement and sampling error. Immeasurable data are initially \textit{guesstimated} from plant experience and their values are subsequently iteratively estimated within the data reconciliation theoretical framework. In this way a dynamic soft-sensor is provided to calculate these data in real-time. At Thermphos International the gaseous product flowrate directly above the furnace, as well as slag and ferrophosphorus flowrates are examples of streams not directly measurable and estimated through data reconciliation. This signals the first step towards the development of a dynamic model. Basic reconciliation theory can be found in Appendix A.

5.3.1 The powerful role of data availability and integrity

Although data reconciliation can be an exceptionally powerful tool, it can only always be as reliable as the data it uses to perform the reconciliation. If, to start with, the data are of poor quality and/or not available, the reconciliation procedure will always be undercut by a fundamental limit to its effectiveness. Two examples are given to illustrate this.

- Owing to the extremely corrosive nature of the gas, it is not possible to measure this important stream in a continuous and/or on-line way. It is only once the phosphorus has reached the final storage tanks that the amount can be determined. This is an example of the lack of availability of key data and why, as will be seen later, the standard deviations \((\sigma)\) associated with this, and some other streams had to be very high.

- The entrainment of ferrophosphorus drops with the slag phase; when the slag
samples are analysed, the X-ray fluorescence spectroscopy only provides the relative total amounts of each element analysed for and reports everything as oxides. The ferrophosphorus is therefore represented as Fe$_2$O$_3$. This is an example of poor data integrity and the solution is to have a constraint that forces 45% of the iron in the Moeller stream to exit the furnace with the slag stream - an amount known through experience.

Measurement bias is another aspect that may impact significantly on data reconciliation results. It is a type of gross error that could be caused by many sources, such as poorly calibrated or malfunctioning instruments. Process leaks can also be represented by a number of biased measurements. If data corrupted with gross errors are reconciled, the error is spread across all variables, degrading the quality of the estimates. It is therefore apparent that some prior knowledge of the system is required before any reconciliation can be done. Reconciliation without a good metallurgical understanding always leads to erroneous results. One way of decreasing erroneous results, as well as detecting and eliminating measurement bias is through the identification and removal of outlier values.

5.3.2 Outlier criteria

On metallurgical plants mistakes invariably creep into the data and it is important to identify these values and deal with them accordingly. The data must therefore be examined for unrealistic values and discrepancies brought on by practical process limitations, analytical limitations and human error. If these values were accepted uncritically, they would have devastating effects on the estimated reconciliation (and estimated model) results. The reason is that quadratic criteria of Equation A.1 give an unreasonably large weight to data points that give large prediction error. Segments that contain inaccurate or doubtful measurement values should be avoided. If this is impossible, the inaccurate values could be smoothed by hand to interpolated or predicted values. The following filter criteria were enforced over the above-mentioned data:

- All data where Fe$_2$O$_3$(slag) wt% were ≥ 2 wt%, were smoothed - thus not allowing the P in entrained ferrophosphorus drop in the slag to contaminate the P$_2$O$_5$(slag) data.
- All data associated with the timestamp where total Moeller flowrate was ≤ $23\text{[ton/mo}un\text{s}]$ were removed - effectively removing down-times from the data set.
- All data where P$_2$O$_5$(slag) were ≥ 4 wt% were interpolated by hand - thus not allowing burden collapses and subsequent rise in unreduced P$_2$O$_5$(slag) loss with the slag just before slag sampling to influence results.

5.3.3 Input and output streams, stream elements and standard deviations

The reconciliation of the process was done in two parts. Figure 5.7 gives a flowsheet of the process and clearly indicates the area around which reconciliations were performed.
Part 1 is around the furnace itself. The five input streams are pellets, coke, silica gravel, electrode (as a result of erosion) and sludge. The three output streams are slag, ferrophosphorus and the gaseous product stream. The elements that are reconciled in every stream are P, Ca, Si and Fe.

Part 2 is around the downstream equipment and the gaseous product stream links the two parts together, with the difference that the gaseous product stream is now the only input stream. The four output streams are \( P_4 \), the additional gas (from hereon referred to as FOG), the dust particles accumulated in the electrostatic precipitators and the sludge from the filters (this becomes an input to the first part). The elements that are reconciled in every stream are P, Ca, Si and Fe.

All of the streams seen in Figure 5.7 have \( \sigma \) values that reflect the quality of the measurements of each particular stream. As also seen from Equations A.1 and A.2, the \( \sigma \) value is required for every stream in order to construct the total objective function and perform the minimisation thereof. Table 5.2 gives the \( \sigma \) values for each element in each stream. The following comments pertain to Table 5.2:

- The \( \sigma \) values associated with the total flowrates of the pellet, coke and silica gravel streams is very small. The reason is the high level of accuracy obtained with the radio active density measurements at the weighing stations.

- The \( \sigma \) values for the elements associated with the pellet stream are, therefore, also very small. The reason for this is the high level of accuracy obtained with the XRF spectroscopy.

- All \( \sigma \) values associated with the gaseous output stream are very high. The reason for this has been explained before - the stream is not directly measured and must be allowed to fluctuate during the optimisation process.
5.3 Data reconciliation

- The σ values for the elements associated with the coke and silica gravel streams are bigger than the pellet stream values. Although these measurements are also performed with the XRF spectroscopy, they are sampled and measured less frequently.

- The other σ values were not quantified but obtained through plant expertise and trail-and-error.

Table 5.2: The standard deviations associated with each element in every stream connected with the data reconciliation

<table>
<thead>
<tr>
<th>Stream</th>
<th>Symbol flowrate</th>
<th>Total stream (Θ)</th>
<th>P</th>
<th>Ca</th>
<th>Si</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pellets</td>
<td>m Pe</td>
<td>0.5%</td>
<td>0.5%</td>
<td>0.5%</td>
<td>0.5%</td>
<td>0.5%</td>
</tr>
<tr>
<td>Coke</td>
<td>m C</td>
<td>0.5%</td>
<td>-</td>
<td>10%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Silica gravel</td>
<td>m Sp</td>
<td>0.3%</td>
<td>-</td>
<td>20%</td>
<td>1%</td>
<td>50%</td>
</tr>
<tr>
<td>Electrode</td>
<td>m E</td>
<td>1%</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Sludge</td>
<td>m SI</td>
<td>10%</td>
<td>10%</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Slag</td>
<td>m Slag</td>
<td>10%</td>
<td>16% (Table 3.6)</td>
<td>0.5%</td>
<td>10%</td>
<td>10%</td>
</tr>
<tr>
<td>Ferrophosphorus</td>
<td>m Ferro</td>
<td>2.5%</td>
<td>5%</td>
<td>-</td>
<td>5%</td>
<td>5%</td>
</tr>
<tr>
<td>Gaseous product</td>
<td>m GP</td>
<td>50%</td>
<td>25%</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>P4</td>
<td>m P4</td>
<td>10%</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Additional gas</td>
<td>m FOG</td>
<td>10%</td>
<td>10%</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Dust</td>
<td>m D</td>
<td>10%</td>
<td>10%</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

5.3.4 Constraints and element balances

The constraints used for the reconciliation can be divided into two groups:

Material conservation constraints  Conservation of mass, and this case elemental flowrate, is the most important component. The material constraints associated with Part 1 of the reconciliation process are:

\[
(m_{Pe} \cdot \Theta) + (m_{C} \cdot \Theta) + (m_{Sp} \cdot \Theta) + (m_{E} \cdot \Theta) + (m_{S} \cdot \Theta) - (m_{Slag} \cdot \Theta) - (m_{Ferro} \cdot \Theta) < 0.1
\]  (5.2)

\[
(m_{Pe} \cdot P) + (m_{Sp} \cdot P) - (m_{Slag} \cdot P) - (m_{Ferro} \cdot P) - (m_{GP} \cdot P) < 0.1
\]  (5.3)

\[
(m_{Pe} \cdot Ca) + (m_{Sp} \cdot Ca) - (m_{Slag} \cdot Ca) < 0.1
\]  (5.4)

\[
(m_{Pe} \cdot Si) + (m_{C} \cdot Si) + (m_{Sp} \cdot Si) - (m_{Slag} \cdot Si) - (m_{Ferro} \cdot Si) < 0.1
\]  (5.5)

\[
(m_{Pe} \cdot Fe) + (m_{Sp} \cdot Fe) - (m_{Slag} \cdot Si) - (m_{Ferro} \cdot Si) < 0.1
\]  (5.6)

The material constraints associated with Part 2 of the reconciliation process are:

\[
(m_{GP} \cdot \Theta) - (m_{P4} \cdot \Theta) - (m_{FOG} \cdot \Theta) - (m_{SI} \cdot \Theta) - (m_{D} \cdot \Theta) < 0.1
\]  (5.7)

\[
(m_{GP} \cdot P) - (m_{P4} \cdot P) - (m_{SI} \cdot P) - (m_{D} \cdot P) < 0.1
\]  (5.8)
There is also another material constraint involving the phosphorus balance that transcends the two parts to ensure their overall integrity:

\[(m_{Pe} \cdot P) - (m_{Slag} \cdot P) - (m_{Ferro} \cdot P) - (m_{P4} \cdot T) - (m_{D} \cdot P) < 0.1 \quad (5.9)\]

Notice that the sludge stream is recycled back to the furnace and therefore not included in this last constraint. A criteria of 0.1 was used for all the equations, a value accurate enough for a metallurgical application.

**Split factors** The second group of constraints makes sure that certain composition ratios or split factors are adhered to throughout the reconciliation exercise. One example is the iron split between slag and ferrophosphorus mentioned in Section 5.3.1. All split factors associated with both parts are as follows:

- The measured basicity of the slag (e.g. 0.88 \([\frac{SiO_2}{CaO}]\) wt%) is assumed accurate and the reconciled slag basicity is not allowed to deviate from this value with more than a standard deviation of 11.3% (e.g. 0.88 ± 0.1)

- In Section 2.9.2 it shows that the ferrophosphorus contains between 15 and 28 wt% P, corresponding approximately to the formula Fe\(_2\)P and FeP. The reconciled ratio is not allowed to deviate outside this range.

- Experience at Thermphos International has shown that 45% of the iron that enters with the Moeller is entrained with slag as ferrophosphorus droplets. The reconciled data are not allowed to deviate from this value with more than a standard deviation of 11.1% (45% ± 5%).

In Appendix B there are a series of screen captures depicting the Excel sheets used for the reconciliation process.

### 5.3.5 Reconciliation results

The data utilised for reconciliation pertain to Furnace 1 and is from 22 August 2005 until 10 May 2006. The data were reconciled according to the principles described in previous sections. The elements that were reconciled are P, Ca, Si and Fe. In the fist reconciliation part, these elements were reconciled for the pellets, coke, silica gravel and sludge streams, together with the gaseous product, slag and ferrophosphorus streams. In the second reconciliation part, these elements were reconciled for the feed stream gaseous product, together with the product streams \(P_4\), additional gas, sludge and dust. The reconciliations were all performed using the Generalised Reduced Gradient (GRG) error minimisation algorithm briefly described in Appendix A.

Figure 5.8 shows the actual vs. the reconciled basicity in the slag for the period from the 1st September to the 31st of October 2005. Figure 5.9 shows the reconciled phosphorus flowrates of the streams (Equation 5.9) for the month of September 2005. After reconciliation, the total phosphorus flowrate in the pellet stream corresponds
5.3 Data reconciliation

Figure 5.8: The actual vs. the reconciled basicity in the slag for the month of September 2005.

Figure 5.9: The reconciled phosphorus flowrates seen in Equation 5.9 for the month of September 2005.

very closely to the sum of the phosphorus contained in the slag, ferrophosphorus, dust and final product streams. The flowrate of the final phosphorus stream is not directly measured, but is now estimated in a real time way.
5.3.6 Soft-sensors estimation and their role in cost analysis of furnace operations

In order to obtain a true picture of optimum furnace operating conditions, the information about e.g. the phosphorus losses in the slag must be contextualised with the flowrate of slag. This will be done together with information about the purchase price of feed material, electrical costs and selling prices of product streams. To make all this possible, the data reconciliation was performed to obtain flowrates not directly measured at Thermphos International. Through the data reconciliation, certain product streams and their flowrates could be estimated (within the set of constraints set out in Section 5.3.4) and utilised in the subsequent profitability study. These streams include:

- The gaseous product flowrate including the $P_4$ flowrate
- The slag flowrate
- The ferrophosphorus flowrate

Figure 5.10 depicts the values of these streams as obtained through reconciliation for September 2005. Therefore, the data reconciliation exercise provides a dynamic soft-sensor to estimate these streams, as well as specific power consumption (SPC) in real-time. Data reconciliation has also prepared the data for dynamic model development.

![Figure 5.10: Gaseous product, $P_4$, slag and ferrophosphorus flowrates obtained through data reconciliation for September 2005.](image-url)
5.4 Optimal furnace operating conditions as identified through cost analysis

5.4.1 Introduction

As defined by The Data Management Association (2007), cost analysis is a systematic approach for identifying, summing and reporting the actual costs of a particular process - in this case the submerged arc furnace. Cost analysis focuses on three major types of costs. These are up-front costs, back-end and operating costs:

- Up-front costs comprise the initial investments and expenses necessary to implement the phosphorus furnaces. These include public education and outreach, land acquisition, permitting, building construction or modification etc. These cost will not be included in this cost analysis exercise.

- Back-end costs include expenditures to properly wrap up operations and take proper care of facilities at the end of their useful lives. Costs include site closure, building/equipment decommissioning, postclosure care, and retirement/health benefits for current employees. Thermphos International is still operational and these cost can not be included in the cost analysis exercise.

- Operating costs are the expenses of managing a submerged arc furnace on a daily basis, including operations and maintenance, capital costs, debt service, and any unexpected costs. Operating costs fall into two broad categories; fixed costs, which are the same whether the furnace is shut down or running at 55MW capacity and variable costs, which may increase depending on whether more production is done and how it is done.

5.4.2 Cost analysis streams and calculations

Actual cost of the streams were used in obtaining the results in this section but, because of their sensitivity, are not mentioned in this report. The variable costs alone are considered here and the following costs streams will be utilised:

- Moeller material costs; apatite, cokes, silica gravel and their corresponding mass flowrates [per day].

- Electricity costs and the MWh utilised [per day]

- Selling prices; P₄, slag, ferrophosphorus, CO and their corresponding mass flowrates [per day]

- The mass flowrates of P₄ losses through the slag and the ferrophosphorus [per day]

There are some material costs associated with the process that are not considered e.g. cooling water and gaseous phosphorus condensation water. All electrical, maintenance and operating cost for the upstream as well as downstream equipment are also not included. Examples of these are the dezincing unit, the granulator
disks, the electrostatic precipitator, the filtration unit etc. The aim of this cost analysis exercise was therefore not to present a total cost estimate of the whole process chain but to identify which operational range of the furnace is the most profitable. This against the background that, while the SPC and the $P_4$ production rate graphs indicated in Figure 5.6 show the same operational range of maximum profitability, the $P_4$ recovery and $P_{\text{slag}}$ graphs report maximum $P_4$ losses around the same area. The following calculations were performed:

**Expenses on a daily basis**

\[
\frac{\$\text{Moeller}}{\text{day}} = \left( \frac{m_{\text{Pellets}}}{\text{day}} \cdot \frac{\$\text{Pellet}}{\text{ton}} \right) + \left( \frac{m_{\text{Coke}}}{\text{day}} \cdot \frac{\$\text{Coke}}{\text{ton}} \right) + \left( \frac{m_{\text{Silica}}}{\text{day}} \cdot \frac{\$\text{Silica}}{\text{ton}} \right)
\]

\[
\frac{\$\text{Electricity}}{\text{day}} = \left( \frac{\text{MWh}}{\text{day}} \right) \cdot \left( \frac{\$\text{Electricity}}{\text{MWh}} \right)
\]

\[
\frac{\$P_4[^{\text{loss}}]}{\text{day}} = \left( \frac{m_{P_4[^{\text{Slag}}]} + m_{P_4[^{\text{Ferro}}]} + m_{P_4[^{\text{Gas}}]}}{\text{day}} \right) \cdot \left( \frac{\$P_4}{\text{ton}} \right)
\]

**Income on a daily basis**

\[
\frac{\$\text{Output}}{\text{day}} = \left( \frac{m_{P_4}}{\text{day}} \cdot \frac{\$P_4}{\text{ton}} \right) + \left( \frac{m_{\text{Slag}}}{\text{day}} \cdot \frac{\$\text{Slag}}{\text{ton}} \right) + \left( \frac{m_{\text{Ferro}}}{\text{day}} \cdot \frac{\$\text{Ferro}}{\text{ton}} \right) + \left( \frac{m_{\text{CO}}}{\text{day}} \cdot \frac{\$\text{CO}}{\text{ton}} \right)
\]

**Profitability on a daily basis** (by using Equations 5.10, 5.11, 5.12 and 5.13)

\[
\frac{\$\text{profit}}{\text{day}} = \left( \frac{\$\text{Output}}{\text{day}} \right) - \left( \frac{\$\text{Moeller}}{\text{day}} \right) - \left( \frac{\$\text{Electricity}}{\text{day}} \right) - \left( \frac{\$P_4[^{\text{loss}}]}{\text{day}} \right)
\]

In Equation 5.14 $\frac{\$\text{profit}}{\text{day}}$ represents the profitability on a daily basis.

### 5.4.3 Cost analysis results

Figure 5.11 shows the daily profitability of this particular furnace [per day] over the operating range described in Figure 5.1 and by using Equation 5.14. It is clear that even with the additional $P_4$ losses associated (Moeller flowrates $\geq$ 25-30 [ton/hour] AND C-fix $\leq$ 0.475) included in the calculations, the decreased electricity cost and not decreased $P_2O_5^{\text{slag}}$ remains the more dominant factor. This shows that the drive for lower SPC and not higher $P_4$ recovery should be getting top priority. It is in this area that the highest profit margins are obtained.
5.5 Conclusions

The common practice of compensating for increased $P_2O_5_{(slag)}$ by increasing the C-fix in the packed bed has limited effects over the long term.

At constant Moeller flowrates, $P_2O_5_{(slag)}$ values were largely independent of C-fix and mostly a function of residence time.

$\tau_{tot}$ is the most influential variable responsible for conditions in the furnace. However, it is not possible to simply adjust the residence time in order to increase SPC.

A C-fix = 0.41 is thermodynamically capable of reducing all the $P_2O_5$ present in the Moeller feed.

The SPC is at a minimum in the area where Moeller flowrates are $\geq$ 25-30 AND C-fix $\leq$ 0.475 - in other words, at high Moeller flowrate AND low C-fix!

Data reconciliation is a powerful tool to close mass balances. It also acts as a dynamic soft-sensor to estimate stream flowrates and SPC not directly measured on the plant. Data reconciliation also prepares the data for dynamic model development.
- The drive for lower SPC and not higher P₄ recovery (less P₂O₅(slag)) should be getting top priority.

The next step towards the creation of the dynamic-CFD hybrid model is to use the identified, cleaned and reconciled data in this chapter in order to choose an appropriate model with which to continue.
Chapter 6

The fluctuating state of the furnace and its influence on data structuring and dynamic model selection

A phosphorus producing, submerged arc furnace is continuously fluctuating between a dynamic-driven state and a thermodynamic-driven state. The detection of this was made possible by the division of data into flowrate-, composition- and electrical data groups and quantifying each group’s influence on the model’s output variable. A linear and a non-linear model were tested, with both type of models showing similar predictive accuracies. The reason for this is the fluctuating state of the furnace where non-linear models are more equip to deal with thermodynamic non-linearities but linear models can perform well with dynamic-driven systems far away from thermodynamic equilibrium. An adaptive, linear, ARX-type dynamic model in discrete time was chosen as the dynamic part in the dynamic-CFD hybrid model.
6.1 Introduction

Normally, in any metallurgical furnace that operates with a heel (an industry term for the residual amount of a specific melt phase - alloy, matte or slag - that remains after tapping) and batch tapping, the process is often dominated by the furnace’s drive to reach thermodynamic equilibrium within its own boundaries. Non-linear techniques can then be employed to model the process (Eksteen, 2004). However, continuous gravitational feed, continuous tapping of the slag and the insignificant heel associated with the phosphorus process causes the furnace to operate without ever reaching equilibrium. It is during this dynamic-driven state that linear techniques also show some potential as a predictive tool. In order to highlight this fluctuating nature of the phosphorus furnace, Chapter 6 uses unique data structuring. It does this by developing preliminary models using both linear- and non-linear techniques on similar data sets and comparing the outcomes. The result is an informed choice on the specific dynamic model which will form part of the eventual dynamic-CFD hybrid model.

The ultimate aim of the dynamic-CFD hybrid model is to minimise energy consumption. It will do this through its ability to predict future outputs one time step in the future; then taking the necessary control action in order to steer these process outputs within given setpoints and product quality constraints. This chapter will therefore also introduce some of the considerations when developing a dynamic (prediction) model.

6.2 The prediction challenge

The objective of any prediction exercise is to determine the future values of a variable based on the available information. The more representative the information, the better is the chance for producing close predictions. Unfortunately it has to be said that the best prediction is that the prediction cannot be the best. This is because, in real life, bestness cannot be precisely measured. Predictions depend on the aspects that include data or measurements available, the system generating the data, the environment influencing the measurements, the dynamic state of the system and the prior subjective knowledge of the process. There is a possibility of inaccuracy or imprecision with each of these. So a sensible objective will be to generate meaningful predictions. The basic issues involved are discussed below and, unless stated otherwise, Kanjilal (1995) was used as reference.

Representativeness of the data  The observations or measurements obtained from the process may be contaminated with noise (error), because the variable concerned may not be directly or precisely measured. An example of this is the slag stream where it was determined that $P_2O_5(slag)$ had a standard deviation of 16% (see Section 3.5). It is therefore vital to understand that any suggested model, no matter how complex and intricate, will have an adopted uncertainty to its prediction, one that can only be decreased by a change in sampling practice.
Modelling versus Prediction  A model, which appears to fit the data well, may not necessarily be able to produce meaningful predictions. In fact, with increased model order (past values), it is always possible to get a closer fit with the data used to generate the model. The model fit against a separate block of data, not used for developing the model, will be a better indication of the validity and predictive accuracy of the model. This block of data are referred to as validation data and if the model is valid irrespective of the choice of validation data within the complete set, it is expected to be able to produce close and meaningful predictions. In this study the following terminologies will be used: (i) Modelling data are the data used to train (develop) the model (equation) and Validation data are the data not used for training (development) of the model and then used to validate (test) the predictive accuracy of the model.

Rate of adaptation  Real life is not constant and static. Hence, as time progresses, adaptation or modification of the parameters of the model will be necessary. In other words, the model (equation) must constantly be updated (re-trained) in order to keep up-to-date on changes in the process. These changes can include the development of freezeline over time, carbon lining erosion, new mixtures of feed material, seasonal changes and maintenance shutdown and relining of a furnace. The validity of the prediction requires the model to be representative and also to remain representative over the period of prediction. It is, therefore, again important to note that the model presented in this report only encapsulates the dynamics of the process over its particular time range.

Prediction and its validity  Once a model is developed, it can be used to produce predictions. There being no single standard method of testing the accuracy of predictions, the chosen method should incorporate the overall sense of the predictions. In this report the accuracy of the prediction is assessed through the coefficient of determination, or $R^2$; where a $R^2$ value of e.g. 0.35 means that the input variables used to train (develop) the model explains 35% of the changes seen in the model output over the data under investigation. A large deviation of the prediction at one single data point (outlier value) can, however, make the cumulative square error too large ($R^2$ too small), irrespective of the prediction being otherwise sensible. So, although $R^2$ is an informative index, it cannot be the only factor for quality or prediction. In fact, a plot of the prediction along with the actual values will provide additional insight into the closeness of the prediction.

6.3 Choosing a dynamic prediction model

The understanding and study of any process, requires a mathematical representation or model of the process. Prediction models that have been developed for different systems can and should have different characteristics depending on the properties of the system and on the mathematical tools used. For representative modelling, the choice of the model, the estimation of parameters and the testing for validity of the model are all equally important. Parameter estimation techniques are not described
in this study, but model validation will be dealt with in detail in Section 9.11. This section briefly lays out the types, as well as candidate classes of models available and describes the thought system involved in choosing a model for the Thermphos International submerged arc furnace process.

6.3.1 Different types of models

A number of adjectives are used to describe the different types of process models (Kanjilal, 1995).

**Deterministic - Stochastic - Adaptive** A process model is deterministic if it works with an exact relationship between measurable and derived variables and expresses itself without uncertainty. Most real-life processes, however, cannot be represented by deterministic models, because of the dynamic nature of the process, the noise (error, lack of information) and other uncertainties being associated with the available data. This means that the description of the process by the model can only be probabilistically close to the actual process and never match it exactly. A model which incorporates noise or distribution terms to try and account for such imprecision in the knowledge of the process is called a stochastic model. If, like at Thermphos International, the characteristics of the process also changes with time, the parameters of the model are to be estimated recursively. Such a model is called an adaptive model and is the type of model used in this study.

**Dynamic - Static** A process (system) is usually characterised by a number of variables that change with time. At Thermphos International these include electrode operating heights, voltage and gaseous outlet temperature to name a few. If these are direct, instantaneous links to variables, the system is static. A resistor is an example of a static system, since the current through it and the voltage across it are directly linked with Ohm’s Law. The current through it depends only on the present voltage and not on earlier values. For other systems the variables can change also without direct outside influence and their values will thereby also depend on earlier signals (variables). Such processes (systems), which include the process at Thermphos International, are called dynamic processes.

**Continuous time - Discrete time** A process model that describes the relationship between time continuous signals (variables) is called time continuous. Differential equations are often used to describe such relationships. In practice, the variables (signals) of interest are most often obtained in sampled form as a result of discrete time measurements. A model that directly expresses the relationship between values of the variables (signals) at the sampling instants (times) is called a discrete time model. Such a process model, which includes the process at Thermphos International, is typically described by difference equations (equivalent to differential equation in continuous time). It is important, however, to remember that the very mathematical definition of a discrete time model is based on the fact that the time between variable observations remains constant!
6.3.2 Different classes of models

Four broad classes of discrete-time, models are mentioned here. They are (1) models based on trigonometric functions, (2) models based on orthogonal transformations, (3) parametric (time series and transfer function) models and (4) hierarchical models that include neural networks. A common feature of these models is that they can all accommodate a certain degree of uncertainty and can adapt to time-varying process dynamics. These models are not discussed here but detailed theory can be found in Kanjilal (1995) and Ljung (1994).

The class of model (linear) chosen for Thermphos International was a parametric model class. This class describes systems in terms of differential equations and transfer functions. Time series is simplified parametric model structures used in the generation of models where outputs are only dependent on previous outputs and disturbances. It may or may not have a periodic associated with it. Time series may be represented by AR, IAR, ARMA, ARIMA (auto regressive integrated moving average) type models. Transfer function models are natural extensions of time series models. It is expected that the process in question is subjected to certain external inputs, which influence output of the system. Transfer functions have additional terms for the exogenous input(s) of which ARX, ARMAX (ARMA with eXogenous input(s)), Box-Jenkins and Output-Error models are examples of. The ARX model is the simplest model incorporating the exogenous input (stimulus signal).

In conclusion, the two classes of dynamic models chosen were a linear model of the transfer function class (ARX structure) and a non-linear model of the rule-based class.

6.4 The concepts of data, data sampling and sampling intervals

Next, the concepts of data, data sampling and sampling intervals are discussed. These concepts are used often in the rest of the book.

Data Data consist of statements that reflect reality. The word data is mentioned throughout this study in different ways. Some data are referred to as past data, while others are future data. In the context of this report the following are the definitions of data:

- Present data, be it input or output data, refer to data sampled at the present time, or \( t = 0 \). In the context of this report, present data will always refer to
as averaged data over the duration of the previous sampling interval up to the present time.

- *Past data* refer to data sampled one or more than one sample interval in the past.

- *Future data* refer to data to be sampled one or more than one sample interval in the future.

**Sampling**   Sampling is another word used in this report. In the signal processing field, sampling is the reduction of a continuous signal to a discrete signal. A common example is the conversion of a sound wave (a continuous-time signal) to a sequence of samples (a discrete-time signal). All data *sampled* at Thermphos International are, however, discrete in nature. In the statistics field, sampling is that part of statistical practice concerned with the selection of individual observations intended to yield some knowledge about a set of entities (data) of concern, especially for the purposes of statistical conclusions. This definition more closely resembles two types of *sampling* defined below:

- In the Thermphos International context, sampling entails the moment when a small amount of e.g. slag is manually extracted by an operator in order to be sent for analyses. This type of sampling will be referred to as *Thermphos-sampling*.

- In the modelling context, sampling is when a model requires certain values at certain times and then selects, or samples, the required value from a actual, Thermphos-sampled data set. To ensure that actual data are available at every sample instant, the discrete Thermphos International data must be converted to a continuous data set. The transformation from discrete to continuous was done by a zero-order hold mathematical model. The zero-order hold is a model of the practical signal reconstruction done by a conventional digital-to-analog converter. That is, it describes the effect of converting a discrete-time signal to a continuous-time signal by holding each sample value for one sample interval. This type of sampling will be referred to as *model-sampling* and was performed for this study by using *MATLAB* (2007).

**Sampling interval**   This refers to the time between two sampling event - be it Thermphos-sampling or model-sampling. Now, it is important to fully understand the concepts of a dynamic-driven state and a thermodynamic-driven state

### 6.5 The concept of a furnace state

The term state can also be used as a synonym for a moment in time, a point of time, a single instant. Since the furnace as a whole can be considered a system of particles, we can speak of the state of the furnace.
6.5.1 A thermodynamic-driven state

In thermodynamics, a thermodynamic state, or more precisely, a macrostate, can be thought of as an optimal ensemble of thermodynamic parameters namely temperature, pressure, density and composition (like the values in Table 6.2), which characterize the system, but neither by its surroundings nor by its history. An example of this is the equation of state that describes the relationship between macrostates of the system. A thermodynamic-driven state (TDS) is when the drive to reach thermodynamic equilibrium within the boundaries of the system, or furnace, is the overriding factor controlling the state of the system. With the submerged arc furnace, such a complete thermodynamic-driven state can exist (theoretically) if all input and output flow are blocked and the contents of the furnace allowed to react for an infinite amount of time within a closed system. Mathematically this can be expressed as:

\[
\text{TDS} = \lim_{x \to \infty} f(x) = \lim_{\tau_{\text{tot}} \to \infty} \text{[State of the furnace (}\tau_{\text{tot}}\text{)]} \tag{6.1}
\]

6.5.2 A dynamic-driven state

In the study of dynamical systems, a physical system is typically modelled as a differential equation. The variable in such an equation is also often called the state of the system. Furthermore, a differential equation is a mathematical equation for an unknown function of one or several variables which relates the values of the function itself and of its derivatives of various orders. Differential equations arise in many areas of science and technology, whenever a deterministic relationship involving some continuously changing quantities and their rates of change (e.g. flowrate variables from Table 6.1) is known or postulated. A dynamic-driven state (DDS) is when the dynamics of these changing quantities supersedes the influence of the drive for thermodynamic equilibrium and is the overriding factor controlling the state of the system. With the submerged arc furnace, such a complete dynamic-driven state can exist (theoretically) if the residence time of the Moeller inside the furnace becomes infinitely small. Mathematically this can be expressed as:

\[
\text{DDS} = \lim_{x \to 0} f(x) = \lim_{\tau_{\text{tot}} \to 0} \text{[State of the furnace (}\tau_{\text{tot}}\text{)]} \tag{6.2}
\]

6.6 Reconciled data structuring in view of choosing a dynamic model

The next section reveals how the reconciled data were structured. The data pertain to Furnace 1 at Thermphos International and are from 22 August 2005 until 10 May 2006. The data were structure into three variable groups and can be seen in Tables 6.1 to 6.3. These data were sampled in different ways as well as at different sampling intervals. In total 17 variables were chosen as input variables. The significance of
The fluctuating state of the furnace and its influence on data structuring and dynamic model selection

Table 6.1: Flowrate data utilised in the prediction model.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>$t - \frac{1}{1}$ sampling interval</th>
<th>$t$</th>
<th>$t + \frac{1}{1}$ sampling interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>F-Moeller</td>
<td>The flowrate of Moeller entering the furnace</td>
<td>[ton/hour]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>F-MWh/F-Moeller</td>
<td>The MWh to F1 ratio</td>
<td>[MWh/F-Moeller]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
</tbody>
</table>

Table 6.2: Composition data utilised in the prediction model.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>$t - \frac{1}{1}$ sampling interval</th>
<th>$t$</th>
<th>$t + \frac{1}{1}$ sampling interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-Mn</td>
<td>The amount of Mn in slag</td>
<td>[wt%]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-Ti</td>
<td>The amount of Ti in slag</td>
<td>[wt%]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-Si</td>
<td>The amount of Si in slag</td>
<td>[wt%]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-Bas</td>
<td>The ratio of $\text{SiO}_2$ and $\text{CaO}$ in slag</td>
<td></td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-fix</td>
<td>(see Section 2.11.1)</td>
<td></td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-$\text{P}_2\text{O}_5$(slag)</td>
<td>The amount of $\text{P}_2\text{O}_5$(slag)</td>
<td>[wt%]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-Bas/M</td>
<td>The ratio of $\text{SiO}_2$ and $\text{CaO}$ in slag</td>
<td></td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-$\text{P}_2\text{O}_5$(slag)/M</td>
<td>The amount of $\text{P}_2\text{O}_5$(pellet)</td>
<td>[wt%]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-Gravelfactor</td>
<td>(see Section 2.11.3)</td>
<td></td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>C-Cokefactor</td>
<td>(see Section 2.11.2)</td>
<td></td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
</tbody>
</table>

Table 6.3: Electrical data utilised in the prediction model.

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>$t - \frac{1}{1}$ sampling interval</th>
<th>$t$</th>
<th>$t + \frac{1}{1}$ sampling interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>E-TempA</td>
<td>Temperature of gaseous product in outlet A</td>
<td>[K]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-TempB</td>
<td>Temperature of gaseous product in outlet B</td>
<td>[K]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-oh-L</td>
<td>Operating height of the left electrode (see Section 3.2.3)</td>
<td>[m]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-oh-M</td>
<td>Operating height of the middle electrode (see Section 3.2.3)</td>
<td>[m]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-oh-R</td>
<td>Operating height of the right electrode (see Section 3.2.3)</td>
<td>[m]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-mohm-L</td>
<td>Electrical resistance under-left electrode (see Section 3.2.1)</td>
<td>[mΩ]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-mohm-M</td>
<td>Electrical resistance under-middle electrode (see Section 3.2.1)</td>
<td>[mΩ]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
<tr>
<td>E-mohm-R</td>
<td>Electrical resistance under-right electrode (see Section 3.2.1)</td>
<td>[mΩ]</td>
<td>$\times$</td>
<td>$\times$</td>
<td>$\times$</td>
</tr>
</tbody>
</table>
6.7 Phosphorus concentration in slag \( (P_2O_5_{\text{slag}}) \) as model output variable

the amount of \( \times \)'s associated with every variables, involves the history of data in a discrete system. As stated by Scheepers, Yang, Reuter and Adema (2006), a distinction was made between flowrate data, composition data and electrical data:

- **Flowrate data** refer to data only related to the movement of material in and out of the furnace. Flowrate data are measured every second and updated within the database of the plant.

- **Composition data** refer to wt% type data associated with the Moeller, slag and ferrophosphorus streams. Updated composition data are obtained after every Thermphos-sampling interval.

- **Electrical data** refer to the accurate and online data, constantly measured and updated within the database of the plant.

By grouping the data in this way the influence of each of the three data groups on the process could be quantified. If during a particular timeframe, the flowrate data have the biggest quantifiable influence on the output variable the process could be characterised as dynamic-driven. If, however, the composition data have the biggest influence on the output variable the process could be characterised as thermodynamic-driven. If the variables of all three groups were influential, the state of the furnace would be fluctuating from one state to the other. Graphical depictions of this can be seen in Figures 6.2 to 6.8. All the variables can be seen in Tables 6.1, 6.2 and 6.3. Except for C-Mn and C-Ti, all input variable data from Tables 6.1 and 6.2 have been reconciled. The electrical variable data in Table 6.3 were not reconciled. Section 6.10 can now show how reconciled data structured in this way, can reveal the furnace’s fluctuating state. Both classes of models - linear and non-linear - will be used and compared to each other in order to determine which best predicts the output variable. First, however, the choice of \( P_2O_5_{\text{slag}} \) as the output variable of all subsequent models is explained.

6.7 Phosphorus concentration in slag \( (P_2O_5_{\text{slag}}) \) as model output variable

Essentially, phosphorus producers are slag producers, with the mass ratio between slag and \( P_4 \) produced typically lying at around 7:1. Owing to this large production volume of slag, a small amount of \( P_2O_5_{\text{slag}} \) in the slag results in substantial losses of unreduced, potential product. Chapter 5, however, showed that decreasing the \( P_2O_5_{\text{slag}} \) does not necessarily guarantee profitable operation. Yet, the \( P_2O_5_{\text{slag}} \) remains indicative of the fluctuating state of the furnace and chapter 5 also established its correlations with the SPC, phosphorus recovery and, most importantly, the residence time. It is also an output variable directly measured and although its value has a 16% standard deviation (see Section 3.5), the analyses technique is accurate. It is for this reason that the \( P_2O_5_{\text{slag}} \) value has been chosen as the output variable to be predicted by the dynamic models in this and subsequent chapters.
6.8 Linear modelling

The variables shown in Tables 6.1, 6.2 and 6.3 were utilised in model development and the $P_2O_5(slag)$ was the output variable. The model used was of the transfer function class (ARX structure). The model-sampling interval was 8 hours. Seven prediction models were trained and validated on seven different sets of unseen data, each set representing seven of the months under investigation. This was done by the procedures outlined in Chapter 7. The linear, prediction model explained 30% of the variance in the $P_2O_5(slag)$. The results can be seen in Table 6.4, while Figure 6.1 shows the predicted vs. the actual $P_2O_5(slag)$ values for the month of December 2005.

Table 6.4: Results of linear, prediction model utilising the variables depicted in Tables 6.1, 6.2 and 6.3.

<table>
<thead>
<tr>
<th>Validation data</th>
<th>Validation results ($R^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>September 2005</td>
<td>$R^2=0.28$</td>
</tr>
<tr>
<td>October 2005</td>
<td>$R^2=0.26$</td>
</tr>
<tr>
<td>November 2005</td>
<td>$R^2=0.24$</td>
</tr>
<tr>
<td>December 2005</td>
<td>$R^2=0.41$</td>
</tr>
<tr>
<td>January 2006</td>
<td>$R^2=0.28$</td>
</tr>
<tr>
<td>February 2006</td>
<td>$R^2=0.29$</td>
</tr>
<tr>
<td>March 2006</td>
<td>$R^2=0.34$</td>
</tr>
<tr>
<td>AVERAGE</td>
<td>$R^2=0.30$</td>
</tr>
</tbody>
</table>

Figure 6.1: The predicted vs. the actual $P_2O_5(slag)$ values for the month of December 2005.
Non-linear modelling

No output bias is visible, with the prediction sometimes too high and sometimes too low. The overall trend, however, follows this actual $P_2O_5_{(slag)}$ reasonably well. In order to show that (in the case of the phosphorus producing, submerged arc furnace) linear techniques effectively captures the important underlying trends of the process, non-linear techniques were also utilised to develop a prediction model.

6.9 Non-linear modelling

For all non-linear modelling CSense 3.1 (2004) was utilised. CSense utilises rule induction techniques that form part of a broad subfield of artificial intelligence called machine learning. Machine learning is an important form of intelligent data analysis concerned with the development of algorithms and techniques that allow computers to learn. At a general level, there are two types of learning: deductive and, as mentioned, inductive. Induction or inductive reasoning, sometimes called inductive logic, is the process of reasoning that extract rules and patterns out of massive data sets and in which the premises of an argument are believed to support the conclusion but do not ensure it. It is used to ascribe properties or relations to types based on tokens (i.e on one or a small number of observations or experiences) or to formulate laws based on limited observations of recurring phenomenal patterns. This is done through a set of IF and THEN statements. A complete description of rule induction techniques is beyond the scope of this study and relevant theory can be found in Triantaphyllou and Felici (2006). When developing and building a model in CSense 3.1 (2004), thirty percent of the data points are randomly selected for validation purposes. The same variables shown in Tables 6.1, 6.2 and 6.3 were utilised for non-linear model development and the model trained 41 times. The non-linear prediction model explained 29% of the variance in the $P_2O_5_{(slag)}$. The results can be seen in Table 6.5.

<table>
<thead>
<tr>
<th>Statistics</th>
<th>Test results ($R^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum</td>
<td>$R^2$=0.19</td>
</tr>
<tr>
<td>Maximum</td>
<td>$R^2$=0.46</td>
</tr>
<tr>
<td>AVERAGE</td>
<td>$R^2$=0.29</td>
</tr>
</tbody>
</table>

The non-linear model provided remarkably similar results to the linear model. For the reason why non-linear techniques did not prove more successful than linear techniques one has to look at the fluctuating state of the furnace at various times.

6.10 The fluctuating state of the furnace

This is done by exploring the level of influence each input variable had on the predicted output, in other words, perform a cause analysis. Cause analysis is a class of problem solving methods aimed at identifying the causes of problems or events.
The fluctuating state of the furnace and its influence on data structuring and dynamic model selection

*CSense 3.1* (2004) has the inbuilt capability to perform a cause analysis and quantify the influence level of each individual input to the model. It displays the results in a histogram, or bar graph, an example of which can be seen in Figure 6.2.

![Figure 6.2](image)

**Figure 6.2:** A depiction of the individual influence of the input variables on the predicted $P_2O_5(slag)$ 8 hours in the future by using *CSense 3.1* (2004). At this moment in time the basicity and the Moeller flowrate wielded the strongest influence.

The top part of Figure 6.2 shows the predicted vs. actual output values, while the vertical line show the point in the process for which the cause analysis was performed. The exact time is also indicated. The three groups of data are clearly marked. The benefit of the above-mentioned data structuring can now be seen in our subsequent investigation into the fluctuating state of the furnace.

**Thermodynamic-driven state** On the 4th of March 2006 at 15h01, when the non-linear model predicted the $P_2O_5(slag)$ 8 hours in the future, the variable wielding the biggest influence on the output value predicted by the model was the basicity of the slag (C-Bas). This variable and its corresponding bar is circled in Figure 6.2. The basicity of the slag is part of the composition data group. Its influence in this instance points towards a time during the process where state of the furnace was, in part, driven by an attempt to establish thermodynamic equilibrium. Note that this does not imply that local equilibria existed.

Figure 6.3 shows a time when the silicon wt% in the ferrophosphorus (C-Si), the $P_2O_5(pellets)$ (C-$P_2O_5$ – pellets), the ratio of silica gravel-to-pellets and the
6.10 The fluctuating state of the furnace

Figure 6.3: A depiction of the individual influence of the input variables on the predicted $P_2O_5_{\text{slag}}$ 8 hours in the future by using CSense 3.1 (2004). Here the state of the furnace was, in part, driven by an attempt to establish thermodynamic equilibrium.

Figure 6.4: A depiction of the individual influence of the input variables on the predicted $P_2O_5_{\text{slag}}$ 8 hours in the future by using CSense 3.1 (2004). The high level of influence of titanium wt% in the ferrophosphorus occurred often.

manganese wt% in the ferrophosphorus (C-Mn) had the most influence on the predicted outcome of the model. Thermphos International uses silicon wt% in the ferrophosphorus as an indicator of the degree of phosphate reduction. Notice that the following Figures 6.3 to 6.8 do not have the predicted vs. actual graphs.

Figure 6.4 shows an interval during the process when the titanium wt% in the ferrophosphorus (C-Ti) had by far the most influence on the predicted outcome of the model. In the previous example, C-Si did show a high degree of influence, but this did not happen often. C-Ti and C-Mn provided much better indicators of reduction.

Figure 6.5 shows a cycle during the process where two of the operator tools identified
The fluctuating state of the furnace and its influence on data structuring and dynamic model selection

Operator’s tools

Left electrode

Figure 6.5: A depiction of the individual influence of the input variables on the predicted $P_{2O_5\text{(slag)}}$ 8 hours in the future by using CSense 3.1 (2004). Here the operator tools had high levels of influence.

in Section 2.11 had significant influence on the predicted outcome. Notably, the operating height of the left electrode showed considerably more influence than the other two electrodes. This phenomena was consistent throughout and once again emphasises the asymmetrical process characteristics.

In all four above-mentioned examples given as cycles of a thermodynamic-driven state, the influence of the flowrate of the Moeller (F-Moeller) on the predicted outcome of the model was always observed. The F-Moeller is circled in all four figures. The state of the furnace could, therefore, never be described as 100% thermodynamically driven.

**A mixed-driven state** Figure 6.6 shows a time during the process where each and every input variable, to varying degrees, exercised some influence on the predicted outcome of the model.

**A Dynamic-driven state** Figure 6.7 and Figure 6.8 show a time during the process where the flowrate of the Moeller (F-Moeller) had by far the biggest influence on the predicted outcome of the model.

These histograms only represent a few cycles during the $\approx$ six months under investigation but is a reliable representation of the fluctuating state of the furnace. It can never be classified as 100% thermodynamic-driven or 100% dynamic-driven but rather a mixed-driven regime that oscillates between the two theoretical states. It is exactly this characteristic that allows the process to be modelled equally well with both linear and non-linear techniques.

The following were also observed during the non-linear model development process.

- The operating heights for middle (E-oh-M) and right electrode never exerted
6.10 The fluctuating state of the furnace

Figure 6.6: A depiction of the individual influence of the input variables on the predicted $P_{2}O_{5}^{\text{slag}}$ 8 hours in the future by using CSense 3.1 (2004). During this instance almost every input variable exercised some measure of influence.

Figure 6.7: A depiction of the individual influence of the input variables on the predicted $P_{2}O_{5}^{\text{slag}}$ 8 hours in the future by using CSense 3.1 (2004). The flowrate of the Moeller (F-Moeller) had by far the biggest influence. Close to the same level of influence as the left electrode (E-oh-L). This again proofs the asymmetrical nature of the furnace operation seen in Section 3.2.3.

- At no cycle of the process do the electrical resistances variables substantially influence the predicted outcome. The sampling interval of 8 hours is too long for an averaged value of such an ever-changing parameter to have an important impact.

- The influence of C-fix never becomes the most dominant. This validates the findings of Section 5.2.2.

- Owing to its negligible influence, the temperature of the slag was not even included in the model development (see Section 3.2.2).
The fluctuating state of the furnace and its influence on data structuring and dynamic model selection

Figure 6.8: A depiction of the individual influence of the input variables on the predicted \( P_2O_5(\text{slag}) \) 8 hours in the future by using CSense 3.1 (2004).

- The influence on titanium and manganese in ferrophosphorus (C-Ti, C-Mn) are much more indicative of P reduction than Si.

6.11 Conclusions

- The type of process model chosen to model the submerged arc furnace process at Thermphos International was an adaptive, dynamic model in discrete time.
- The two classes of dynamic models chosen were a linear model of the transfer function class and with the ARX structure and a non-linear model of the rule-based class.
- The linear, prediction model explained 30% of the variance in the \( P_2O_5(\text{slag}) \)
- The non-linear, prediction model explained 29% of the variance in the \( P_2O_5(\text{slag}) \)
- The division of data into flowrate-, composition- and electrical data groups makes it possible for models to show the fluctuating state of the furnace between a thermodynamic-driven state and a dynamic-driven state.
- The fluctuating state of the furnace is the reason why linear modelling techniques provide similar results than non-linear techniques; where non-linear models are more equipped to deal with thermodynamic non-linearities, linear models can perform very well with dynamic-driven system far away from thermodynamic equilibrium.
- An adaptive, linear, ARX-type dynamic model in discrete time was chosen as the dynamic part in the dynamic-CFD hybrid model. Not only does it provide similar results as its non-linear counterpart, but it is robust and easy-to-use.
The next chapter explores the predictive ability of the chosen model, performs a sensitivity analysis on all the important variables, makes a thoughtful evaluation of the meaningfulness of the results and assesses the opportunities for process control.
The fluctuating state of the furnace and its influence on data structuring and dynamic model selection
Chapter 7

Linear, dynamic modelling results and the potential for predictive control

A dynamic prediction model showed an 8-hour-ahead predictive accuracy of 30% (±6%) on future $\text{P}_2\text{O}_5(\text{slag})$ values. This inherent relationship exists owing to the long residence times inside the furnace and the metallurgical memory encapsulated within the input variable. Predictive control possibilities were investigated by simulating the set-points of C-fix and silica gravel factor. These are two fully independent variables used by operators to control the process. This linear, predictive control model showed a slight improvement with an 8-hour-ahead predictive accuracy of 35% (±7%), thus exposing how ineffective present time adjustments are in optimally steering the process to a desired output 8 hours in the future. The reason for this is that there are fundamental design-, sampling- and process restrictions currently associated with the process that will always limit the predictive and especially control accuracy or meaningfulness of any dynamic model. Given these fundamental restrictions, not even the perfect dynamic prediction model will significantly improve on an 8-hour-ahead prediction of 30% (±6%).
7.1 Introduction

Chapter 5 stated that choosing a type and class of dynamic prediction model for the Thermphos International process is influenced by the fluctuating state of the furnace, which continuously alters between a thermodynamic-driven and dynamic-driven state. This phenomena, however, ensures that output predictions with linear model provided coefficient of determination values \( R^2 \) similar to non-linear models. An adaptive, linear, ARX-type dynamic model in discrete time was, therefore, chosen as the dynamic part in the dynamic-CFD hybrid model. Appendix C covers some basic theory about the ARX structure model.

This chapter discusses the history of data and it is shown how the ARX structure model can accommodate the *metallurgical memory* of the furnace in order to improve prediction. By assuming future values of the two variables deemed operator tools, predictive control is simulated in another section. The chapter finishes with a sober assessment of the possibilities for prediction and predictive control given certain fundamental design-, sampling- and process restrictions associated with the production of phosphorus with submerged arc furnaces.

7.2 The dynamic prediction model

The Thermphos-sampling interval for all composition data are approximately 8 hours. This means that the time between process control adjustments are also 8 hours and for this reason a model with an 8-hour model-sampling interval best reflect the current situation at Thermphos.

7.2.1 The history of data

The predictive ability of this model is described in terms of its capability to predict the \( \text{P}_2\text{O}_5\text{(slag)} \) one sampling interval in the future. In order to properly facilitate this objective, it is important to consider the inherent process knowledge contained in data from sampling intervals in the past i.e. the data’s history! Linked to this is the *number* of sampling intervals from the past (historic variables) required for optimum prediction. The number of past values of the same variable used in modelling refers to the order of the model and a mixed order comes about when the model variables do not have the same order.

The ARX model in this report is a mixed order model and the number of sampling intervals associated with each variable is indicated \( (\times) \) in Tables 6.1 to 6.3. These chosen orders were a direct result of the residence time of the material in the furnace. In other words, how long does it take for the sampled pellet material at the top of the feed pipes to exit the furnace as slag through the slag tap hole? In practice, this takes between 8 - 12 hours depending on the state of operation. Individual order choices will now be discussed in terms of the data groups.
7.2 The dynamic prediction model

Composition data - Slag  Continuous tapping ensures that no significant heel of slag is ever present in the furnace. That means that all slag inside the furnace at the present time \((t = 0)\) would, given steady-state operations, not be present in the furnace 8 hours in the future, thus removing all inherent knowledge of recent process history, or *metallurgical memory*. Given this, even present composition data should also be excluded, but the inclusion of present data in the development phase are as a result of unforeseen decreases in the production rate, thereby allowing some threads of present time slag history to remain inside the furnace. Circumstances when this can occur are during a changing of the ladles, sudden Moeller collapses and excessive gaseous outlet temperatures. For this reason, present slag composition data, but not past data, were used in developing (training) the 8-hour model.

Composition data - Ferrophosphorus  Ferrophosphorus is tapped from the furnace every 1000MWh, which translates to roughly once a day. Therefore, after tapping any ferrophosphorus formed from then on, will not only increase in volume but also remain in the furnace for on average 24 hours. This would imply that ferrophosphorus data from as far back as two (8-hour) sampling intervals in the past could still hold vital information when attempting to predict one sampling interval in the future. The ferrophosphorus, however, can only be sampled when tapped. This necessitated the use of zero-order holds on all ferrophosphorus composition data in order to be used in the 8-hour model. Attempts to use these data (from one and two sampling intervals in the past) proved unsuccessful and resulted in overfitting. For this reason, only present ferrophosphorus composition data were used in developing the model. These variables include C-Mn, C-Ti and C-Si in Table 6.2. *All composition data, although in the strict sense of the word output variables, were used as time-delayed, input variables.*

Composition data - Moeller  As a result of analysed composition data, the Moeller feed recipe is changed approximately every 8 hours based on the chemical analysis of the slag in a feedback way. This is done to drive a certain set of output variables measured at the present time \((P_{2O5(slag)})\), slag basicity) back towards its specified setpoints. Section 2.3 shows that this adjusted Moeller feed mixture (or an imaginary trace element representing the adjusted Moeller feed) will only reach the reaction zone after between 6 - 10 hours. Add to this another 2 hours before the, now molten, feed mixture (slag) will exit the furnace. This means that that in some cases where the total residence time is \(\geq 10\) hours, flowrate data from one sampling interval in the past could still pass information about the process to the model. For that reason present Moeller composition data, as well as Moeller composition data from one sampling interval in the past were used in predicting the \(P_{2O5(slag)}\) of one sampling interval in the future.

Flowrate data  For the same reasons as the composition data of the Moeller, present flowrate data, as well as flowrate data from one sampling interval in the past were used in predicting the \(P_{2O5(slag)}\) of one sampling interval in the future. These variables are shown in Table 6.1.


**Linear, dynamic modelling results and the potential for predictive control**

**Electrical data**  Electrical data of Table 6.3 represent averaged values of continuously updated electrical data and not merely sampled values as is the case with composition data. This, however, does not increase the historical significance of electrical data from one sampling interval in the past with regards to the model. For that reason only present electrical data were used in the model.

*In summary, only present data and some past data from one sampling interval in the past were used in the development of the dynamic prediction model.*

### 7.2.2 The development phase and eventual predictive ability of the prediction model

The predictive ability of any model ($R^2$) must be calculated by using previously unseen data, or validation data (Section 6.2). A good rule of thumb is to use between 10 - 20% of the overall data set for validation. Another important aspect of validation data are the choice of which segment of data to use, in other words is it better to use the first 15%, the middle 15% or the last 15% of the data? In a perfectly steady-state process where little changes over time, the calculated $R^2$ will remain the same, independent of the segment of data utilised for validation. To observe whether this choice would have an effect at Thermphos International, seven different models were trained (by estimation of the parameters) and then validated on their seven respective segments of validation data. The validation data and corresponding $R^2$ have already been shown in Table 6.4.

The model could predict 30% of the changes in the output variable. The 6% standard deviation is, in part, due to the fluctuating state of the furnace. At times where the drive for thermodynamic equilibrium inside the packed bed might be more prevalent, the linear model will have less success in capturing the inherent trends in the data (e.g September and November 2005). On the other hand, where the state of the furnace is more dynamic-driven, a linear model will show improved predictive ability (e.g. December 2005).

### 7.2.3 The meaningfulness of the prediction model

The low to moderate $R^2 = 0.30$ should always be seen as only part of the overall sense of the prediction, with the other part being a plot of prediction values along with actual values. Such a plot can already be seen in Figure 6.1 but is reshown in Figure 7.1. Although the model has limited ability in terms of any quantitative predictions, it is clear that the model predictions do follow the overall trend of the data. This ability gives the user confidence to use this adaptive, linear, dynamic model as a tool in order to explore the influence of operator-induced input changes for control purposes. These include the silica gravel factor and C-fix.

### 7.2.4 The influence of the input variables on the predicted output

After having developed the prediction model, the influence of individual inputs on the predicted output can be quantified by looking at the pinned weights (or
7.2 The dynamic prediction model

Figure 7.1: The actual output variable vs. the predicted output variable from the prediction model. December 2005 was used for validation.

Figure 7.2: A depiction of the standardised influence the various input parameters had on predicting the output variable.
coefficients of B in Equation C.3). Their standardised value (divided by the average value of the data set), as well as there mathematical signs, underlines the variable’s influence. An example of this is seen in Figure 7.2; the present flowrate values of the Moeller has the most influence on the predicted output value, while an increase to the Moeller flowrate (F-Moeller in the figure) will result in an increase in the predicted $P_{2O_5(slag)}$. This result corresponds with findings summarised in Figure 5.2, where an increase in Moeller flowrate coincides with an increase in $P_{2O_5(slag)}$.

The following deductions can also be made from Figure 7.2:

- The amount of titanium in the ferrophosphorus (C-Ti in the figure) showed a high level of influence on the predicted $P_{2O_5(slag)}$ wt% value and an increase in the level of Ti will coincide with a decrease in $P_{2O_5(slag)}$ wt%. This means that improved reductive conditions as a results of longer residence times and higher temperatures will not only reduce more Ti from TiO$_2$ but also more P from P$_2O_5$.

- The amount of silicon in the ferrophosphorus (C-Si in the figure) does not provide a good measure of the reductive conditions within the furnace.

- The operating heights for middle (E-oh-M) and right electrode exerted much less influence than the left electrode (E-oh-L) - as also shown by the non-linear model in Section 6.9. This again proves the asymmetrical nature of the furnace operation seen in Section 3.2.3.

- Most of the past data provide less influence on the predicted $P_{2O_5(slag)}$.

- It shows that an increase in C-fix will result in an decrease in predicted $P_{2O_5(slag)}$ value.

7.3 The dynamic predictive control model

The difference between the prediction model and the predictive control model is that the control model allows the user to investigate the level of influence that fully independent, operator changes (future data) will have on the $P_{2O_5(slag)}$ value one sampling interval in the future.

7.3.1 The history and potential of data

Changes made to the silica gravel factor and the C-fix are the two main tools used by the operators to control the process. In order to optimally quantify the level of influence of these changes on the output variable 8 hours in the future, the data of one sampling interval in the future associated with these two variables were used to develop the model. In this way a new set-point was simulated and possible control assessed. Apart from future data from the silica gravel factor and the C-fix, all the other data and their respective orders were used in the same way in developing the model.
7.3 The dynamic predictive control model

Figure 7.3: The actual output variable vs. the predicted output variable from the prediction model and the predictive control model. December 2005 was used for validation.

Figure 7.4: A depiction of the standardised influence the various input parameters had on predicting the output variable for control purposes.
7.3.2 The development, results and control ability of the predictive control model

To find out whether the inclusion of future data or, in other words, desired setpoints, would have an effect on the predictive accuracy of the model, seven new models were re-trained (by estimation the parameters) and then validated on the same seven respective segments of validation data. The validation data and corresponding $R^2$ are listed in Table 7.1.

Table 7.1: The validation data and corresponding $R^2$ values for seven different models.

<table>
<thead>
<tr>
<th>Validation data</th>
<th>Predictive ability of the models ($R^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>September 2005</td>
<td>$R^2 = 0.31$</td>
</tr>
<tr>
<td>October 2005</td>
<td>$R^2 = 0.33$</td>
</tr>
<tr>
<td>November 2005</td>
<td>$R^2 = 0.25$</td>
</tr>
<tr>
<td>December 2005</td>
<td>$R^2 = 0.44$</td>
</tr>
<tr>
<td>January 2005</td>
<td>$R^2 = 0.36$</td>
</tr>
<tr>
<td>February 2005</td>
<td>$R^2 = 0.34$</td>
</tr>
<tr>
<td>March 2005</td>
<td>$R^2 = 0.39$</td>
</tr>
<tr>
<td><strong>AVERAGE</strong></td>
<td>$R^2 = 0.35$</td>
</tr>
<tr>
<td><strong>Standard deviation</strong></td>
<td>0.07</td>
</tr>
</tbody>
</table>

7.3.3 The meaningfulness of the control model

The low to moderate $R^2 = 0.35$ only showed an improvement of 5% on the predictive ability; changes made to the silica gravel factor and the C-fix at the present time have limited influence on the $P_2O_5(slag)$ value of one timestep ahead. This leaves the operators with little leverage in controlling the $P_2O_5(slag)$ 8 hours in the future.

A plot of the results can be seen in Figure 7.3. It is clear that the predictive control model does not perform significantly better than the prediction model in following the trend of the output variable. In fact, the two graphs representing the predictive model output and the predictive control output are barely distinguishable.

7.3.4 The influence of the input variables on the predicted output

Figure 7.4 indicates the relatively low level of influence the operator control variables have on the 8-hour output value of the $P_2O_5(slag)$. There two quantitative weights are shown in black bars and clearly have less influence than present data already in the furnace.

7.4 Conclusions

- The prediction model was developed, tested and then shown to have an 8-hour-ahead predictive accuracy ($R^2$, coefficient of determination) of 30% ($\pm 6\%$) on
future P$_2$O$_5$(slag) values.

- This inherent relationship exists because, at the precise moment of a P$_2$O$_5$(slag) prediction, the furnace already contains the metallurgical memory (input variables to the linear model) needed to ensure that some predictive possibilities will always exist - all as a result of the long residence times in the furnace.

**Metallurgical memory**  The 7-10 hours that the Moeller remains in the furnace before reaching the reduction zone (see Section 2.2) show why dynamic modelling of the phosphorus furnace will always provide some insight to the process. When predicting the P$_2$O$_5$(slag) value 8 hours in the future, the most important and influential information (data) are not passed by input variables about to be calculated and changed, but information (data) carried by input variables already in the furnace!

- Residence time is not a directly adjustable variable but rather a fully dependent variable and a function of an array of interconnected and interactive variables. In fact, this applies to virtually all input variables, re-emphasising the importance of innate metallurgical memory.

- Predictive control possibilities can be explored by simulating the set-points of two fully independent variables used by operators to control the process.

- The operator set-points C-fix and silica gravel factor were simulated and the linear, predictive control model showed only a small improvement with an 8-hour-ahead predictive accuracy of 35% ($\pm 7\%$).

- This highlights how ineffective present time adjustments are in optimally steering the process to a desired output 8 hours in the future. It also shows how difficult even incremental improvements in feed-forward and predictive control can be.

- The reason for this is that there are fundamental design-, sampling- and process restrictions currently associated with the process that will always limit the predictive and especially control accuracy or meaningfulness of any dynamic model.

**Design restrictions**  A residence time of 8-12 hours inside the furnace goes to the very core of why any improvement in the furnace control arrangement at Thermphos International is such a difficult task. A process that calculates new input variable values for the present time - devised to drive a certain set of output variables at the present time (P$_2$O$_5$(slag), slag basicity) to specified setpoints - can not be effective when the adjusted variables will only reach the reaction zone 7-10 hours. The reason for this is that in the unlikely event of 8 hours of trouble free, steady-state furnace operation, the adjusted feed mixture will effectively have only 1 hours (8 hours - 7 hours = 1 hour) to make the operational impact it was devised to do! This effectively defines a fundamental
upper limit to predictive improvement. Control accuracy can, therefore, only ever be oscillating in a range best described as a damage-control range, with the input variables to facilitate process adjustments on a short term basis (≤ 8 hours) already in the furnace. No changes can be made to them.

**Sampling restrictions** The Thermphos-sampling interval is 8 hours. This low sampling interval immediately implies that a significant proportion of the dynamics will be obscured from the model. Added to this is a 16% standard deviation that exists on the $P_2O_5(slag)$ value in the slag samples - the very value the model is to predict! This gives the already low to average $R^2 = 35\%$ value seen in Section 7.3 another dimension of uncertainty. These restrictions can only be alleviated through improved measurement accuracy and shorter Thermphos-sampling intervals.

**Process restrictions** A large randomness, resulting from our lack of knowledge of what happens inside the furnace, exists in the model i.e. many of the influential input variables are not known yet!

**Continuously updated electrical data** These data do slightly improve the predictive accuracy of both the prediction- and predictive control model. However, the large model-sampling interval keeps it from playing an as dominant role as first expected at the start of this project.

**Adaptivity** For the model to remain relevant and up-to-date, the model should be retrained regularly, thereby remaining adaptive. This effectively means that the dynamic model developed in this study is already out-of-date and in need of revision.

**Non-linear modelling** A non-linear, neural network-class, dynamic model in discrete time does not predict the $P_2O_5(slag)$ 8 hours in the future more effectively than its linear counterpart. This demonstrates the fluctuating state of the furnace between a dynamic-driven and a thermodynamic-driven state (Scheepers, Yang, Reuter and Adema, 2006) and proves that the use of a non-linear model will not bring about a radical improvement in predictive ability.

Finally, the point is made that, given the current status quo of sampling, design and process, even the perfect dynamic prediction model will not significantly improve on an 8-hour-ahead prediction of 30\% (±6\%). This barrier can only be pierced with e.g. tidier and more frequent sampling regimes and other upfront capital investments, a decision that becomes a cost analysis exercise and that can only be taken by the management structure. For recommendations on how to improve predictions, see Section 11.2.

Part IV will be devoted to the CFD part of the dynamic-CFD hybrid model.
Part IV

The CFD MODEL
Chapter 8

CFD process modelling: Theory and methodology

8.1 Introduction

Computational Fluid Dynamics, CFD, is a numerical tool to simulate fluid flow related problems. The development of modern CFD began with the rise of the digital computer in the late 50’s and was mainly applied to aerospace research. In the late 70’s the first commercial software packages became available and CFD also found its application in a wide variety of engineering problems. Today CFD is used in a great deal of research areas such as aerodynamics of aircraft and vehicles, hydrodynamics of ships, power plant (combustion in furnaces, boilers and gas turbines), turbomachinery (flows inside rotating passages), electrical and electronic engineering (cooling), chemical process engineering (mixing and separation, reactor optimisation), buildings (heating, ventilation, wind loading), hydrology and oceanography (flow in rivers, estuaries and oceans), meteorology (weather forecasting) and bioengineering (blood flow in arteries and veins) (Reuter and Yang, 2000).

CFD is also very useful in resource engineering research, where it has been used for most of the unit operations. For some, such as ladle metallurgy or continuous casting of steel, it has already been used for more than twenty years. For other processes, such as submerged arc furnaces, research was done much later but due to its high complexity has not been extensively studied. CFD is used to model e.g. single and multi-phase flows in furnaces, heat and mass transfer or chemical reactions. Some examples of its use in resource engineering are non-ferrous smelting processes (Flash smelting, Hall-Heroult cell, Peirce-Smith converter), iron and steel making (Blast furnace, HIs melt, Basic Oxygen Furnace, Electric Arc Furnace), ladle metallurgy (gas and electromagnetic stirring), continuous casting of steel (tundish, casting mould), off-gas cooling, dust precipitation (waste-heat boilers, cyclones, electrostatic precipitators), hydrometallurgy (stirring tanks, thickeners, tank-house) etc.

Before exploring the fundamental theory underpinning a CFD model of a submerged
arc furnace, a brief history of electric arc modelling is discussed.

8.2 Literature overview of electrical arc furnaces

There are five main types of electric powered furnaces in use: resistance furnaces, arc furnaces, induction furnaces, electron-beam furnaces and plasma furnaces. In resistance furnaces the heat is generated by direct resistance, according to Ohm’s and Joule’s laws, of the charge to the electrical current. Arc furnaces are heated by the arc created between the electrode and the slag layer. In induction furnaces the heat is generated by induction according to Lenz’s, Ohm’s and Joule’s laws. The electron-beam furnace is heated by high energy electrons generated by electron guns. Plasma furnaces are heated by gas-stabilized plasma arcs produced by water-cooled plasma torches (Ullmanns Encyclopedia of Industrial Chemistry, 2000).

The type of furnace modelled in this study is a sub-type of the electric arc furnace. There are two basic types; the electric or open arc furnace (EAF) and the submerged arc furnace (SAF). In the EAF the electrode is hanging above a slag bath, with the arc between the electrode tips and the slag surface. Both AC and DC EAF furnaces are used to produce iron and steel, ferroalloys and some non-ferrous metals. The electrodes in the SAF (alternating current) are submerged in the charge and arcing takes place between the electrode tips and the slag surface underneath the charge layer. In a SAF the heat is also generated by the resistance of the charge to the electrical current. The SAF is used to produce ferroalloys (Cr, Mn), non-ferrous metals and non-metals (phosphorus, CaSi₂, CaC₂).

The physical and chemical processes in arc furnaces are very complex due to the interaction between electromagnetism, multi-phase fluid flow, heat transfer and heterogeneous chemical reactions. Studies have been conducted in modelling different aspects of arc furnaces for metals production, such as arc behaviour and gas, slag and molten metal flow. The transport phenomena in an electric powered furnace can be classified into two regions:

- The gas region, both free flowing as well as through a packed bed, where electric arcs dominate the fluid flow and energy transport.

- The molten slag, matte or metal region, where there are influences by factors like jet momentum transfer from the arcs above the bath, electromagnetic forces and Joule heating, natural convection due to the temperature gradient, gas bubbling from oxygen lancing or gas generation by chemical reactions and free surfaces between gas/slag and slag/metal.

8.2.1 Electric or resistance furnace

Most studies about electric furnaces investigates the second region; with exceptions like Reynolds (2002) who investigated radiative heat losses of the slag surface to the furnace roof and Guo and Irons (2005) who investigate radiation modelling in an
EAF. Choudhary and Szekely (1981) calculated the electromagntical force fields, velocity fields and temperature fields with a 2D mathematical model. This was done for three electrical systems; electric slag refining (ESR), electric slag welding (ESW) and submerged resistance furnace. An example of their work is shown in Figure 8.1.

![Figure 8.1: Computed isotherms and velocity distribution of ESW unit (Choudhary and Szekely, 1981).](image)

Sheng and Irons (1998) investigated the transport phenomena in nickel matte smelting using a 3D model solved with PHOENICS CFD code. Distribution of electrical potential, heat release, temperature and velocity in slag and matte was calculated; results for the last two are shown in Figure 8.2.

![Figure 8.2: Results of computations for no gas injection and 600 W power input. Top: Velocity vectors. Bottom: Isotherms in degree C. The dashed line indicates the slag/matte interface (Sheng and Irons, 1998).](image)

The furnace was also physically modelled with oil and an aqueous calcium chloride
solution representing the slag and matte. A slag cleaning furnace in the Mitsubishi copper process was modelled by Hasegawa and Kaneda (2000), also in PHOENICS. The research focused on electric field analysis, heat and fluid flow, particle tracking of matte droplets in the slag, and effects of various conditions such as furnace shape and scale, electrode configuration and immersion depth, and thickness of the slag layer. Xia and Ahokainen (2004) and Xia, Ahokainen and Kankaanpaa (2004) modelled slag flow and nickel droplet settling and the effect of electrode immersion depth on it; in a slag cleaning furnace with CFX4 code and user subroutines for magnetohydrodynamics. The governing equations for mass, momentum and energy were solved; while momentum and energy equations were coupled with a set of Maxwell’s field equations and Ohm’s law. An example of their work is shown in Figure 8.3.

![Figure 8.3: Temperature distribution at different electrode immersion depths at 0.3m and 0.6m (Xia, Ahokainen and Kankaanpaa, 2004).](image)

### 8.2.2 Electric or open arc furnace

The electric arc furnace contains phenomena from both regions; literature mostly solves problems for one separate region. Szekely, McKelliget and Choudhary (1983) modelled both arc and melt zones for a steelmaking EAF. The 2D model, however, was simplified by decoupling melt flow and heat transfer from gas flow and heat transfer in the open arc region. The electromagnetic forces and Joule heating were also neglected in the melt zone. Some results are shown in Figure 8.4.

Three phase AC arcs are very complex due to the interactions between the individual electrodes and the periodic changes in the polarity. For that reason, DC arcs are used for simplicity. No attempt was found in literature to model AC arcs directly, except for Larsen, Gu and Bakken (1995) for a SAF AC arc. Qian, Farouk and Mutharasas (1995) modelled a DC arc in an EAF concerning gas flow in the plasma region, and the interaction of thermal energy with the bath surface. Ramirez and Trapaga (2004) and Ramirez, Trapaga and Garduño-Esquivel (2004) used a mathematical model to describe fluid flow, heat transfer and electromagnetic phenomena in the arc region of a DC EAF. The model was
solved using the PHOENICS CFD software. From the results a dimensionless arc description was derived regardless of the values of the arc current and arc length.

Gunnewiek and Tullis (1996) modelled 3D heat and fluid flow in the slag phase of an EAF non-ferrous reduction furnace with Fluent 6.1.18 (2003) CFD code. Thermal energy transferred to (open arc) and generated in (immersed electrode) the slag phase was implemented in the model by heat source blocks. Energy consumption due to melting and reduction reactions was also modelled. Temperature homogenisation in EAF steelmaking was modelled by Caffery et al. (1997) using CFD code TASCflow. The influence of bottom gas bubblers and oxygen lances were investigated; electromagnetic effects on the flow and heating were neglected. Heat transfer from the electrodes to the metal bath was considered. EAF steelmaking was also investigated by Gu and Irons (1999) through a physical oil - water cold model and by a numerical model. The studied phenomena include oxygen lancing, arc jets effect and bottom injection.

8.2.3 Submerged arc furnace

The most complex of electric powered furnaces is the SAF; though region two is quite similar to the EAF, region 1 now also includes chemical reactions, porosity and resistance heating. Larsen, Gu and Bakken (1995) developed a numerical 2D model for an AC arc in a silicon metal SAF using Fluent 6.1.18 (2003). The arc is the main energy source in the furnace (≈90%). The conservation equations for mass, momentum and energy together with time dependent Maxwell’s equation were solved. The model assumes symmetric furnace conditions and takes only one phase in consideration for a 3-phase SAF. Therefore, the significant interactions among phases cannot be reflected by the model. Andresen and Tuset (1997) modelled fluid
flow, heat transfer and heterogeneous chemical reactions above 1850°C in the arc region of a silicon furnace with a 2D Fluent 6.1.18 (2003) model. The AC arc in the gas filled cavity is simplified with a DC arc. The representation of the real furnace in the simulation model is shown in Figure 8.5 and some temperature distribution results in Figure 8.6.

Figure 8.5: The real furnace situation (left) and the 2D model (right) (Andersen and Tuset, 1997).

Figure 8.6: Temperature distribution in the rigid metal pool (left) and in the arc region (right) (Andersen and Tuset, 1997).

Saeardsdottir et al. (2001) investigated arc behaviour in silicon and ferrosilicon furnaces using a 2D model. The behaviour of the solid bed region and overall furnace thermal performance was not included. Sridhar and Lahiri (1994) developed a 2D single electrode model for current and temperature distribution for a SAF for ferromanganese production. Current distribution was calculated by solving Maxwell equations for the magentical field. Joule heating and heat conduction are modelled in the slag and solid zones, the arc and gas flow were not included. Heat sources due to chemical reactions were included. The influence of electrode depth, electrical
8.2 Literature overview of electrical arc furnaces

conductivity of the charge and the slag on power consumption was studied. Ran-
ganathan and Godiwalla (2001) used the same approach for a ferrochromium SAF
furnace to simulate the effects of bed porosity, charge preheat and charge chemistry
on the temperature profile. Some results are shown in Figure 8.7.

Figure 8.7: Temperature profile inside SAF, charge not preheated (left) and preheated to
550°C (Ranganathan and Godiwalla, 2001).

Vanderstaay, Swinbourne and Monteiro (2004) modelled the submerged arc electric
furnace smelting using the manganese-rich slag method process by using the HSC
computational thermodynamics package. It was assumed that higher manganese
and iron oxides are reduced to MnO and FeO before entering the zone where molten
slag and alloy form and equilibrate. The model predictions were compared to data
from Thermit Alloys (P) Limited, an Indian ferroalloy smelter. It was then used to
examine the affects of changing the amount of carbon reductant and temperature
on several performance indicators.

8.2.4 Contributions to CFD knowledge of current study

The transport phenomena of the molten materials have been investigated by many
authors. In this thesis the molten materials are not simulated and, therefore,
leaves three relevant articles; Sridhar and Lahiri (1994), Ranganathan and Godi-
walla (2001) and Vanderstaay, Swinbourne and Monteiro (2004). All three used 2D
models to study current and temperature distribution in the packed bed and slag.
The first two also incorporated Maxwell equations, Joule heating and chemical reac-
tions, but excluding gas flow and arcs. No attempt has been made to develop a 3D
model of a complete furnace to simulate chemical reactions in the packed bed com-
bined with gas generation and flow. The model described in this thesis might not
simulate Maxwell and Joule equations, but it is the first CFD model of a submerged
arc furnace that:

- is completely three-dimensional,
- uses a furnace modelling structure that is 100% exactly the same as the actual
  furnace,
- uses boundary conditions, initial values and material specifications provided by industrial measurements, laboratory experiments and a combination of empirical and thermodynamical data,
- accounts for fully developed gas flows of gaseous product gas not introduced to but generated from within the packed bed through the Wöhler reaction,
- accounts for the energy associated with chemical reactions, heating and melting and phase transformation in the packed bed,
- account for the thermal conductivity and the particle-particle radiation within the packed bed,
- provide an in-depth, case specific CFD model catering to the specific needs of the submerged arc furnace, phosphorus producers and provides real, industrial answer to real, industrial problems and scenarios,
- implements the integration of accurate, multi-field thermodynamical data and kinetic reaction rate data with computational flow dynamic calculations successfully
- takes the unification of the sciences of kinetics and equilibrium thermodynamics to a next level,

The rest of this chapter will look at fundamental knowledge required to built up a CFD model.

8.3 Fundamentals of CFD

There are two types of CFD codes which can be used for solving engineering problems; self-made code or general purpose commercial code. Self-made code requires a great amount of time and knowledge, but can be very efficient in solving a specific problem. In this thesis a general purpose commercial CFD code is used, which has the advantage of well developed and flexible code and saves a great deal of coding time. There are several commercial general purpose CFD packages available on the market. These packages consist of three main components;

- Pre-processor: Geometry creation and meshing
- Solver: Core of the code performing calculations
- Post-processor: Tools to analyse and visualise results

A few well known general purpose codes suitable for PC’s are PHOENICS, Fluent 6.1.18 (2003), ANSYS CFX (2007) and FLOW-3D (2007). These codes use a range of numerical methods, grid systems, physical models and solution techniques. The Fluent 6.1.18 (2003) code is used in this thesis; where Gambit 2.04 (2003) is the pre-processor and Fluent 6.1.18 (2003) the solver and post-processor. In this chapter, unless stated otherwise, the extensive users guide of Fluent 6.1.18 (2003) was used as reference.
8.3 Fundamentals of CFD

8.3.1 Governing partial differential equations

The Fluent 6.1.18 (2003) CFD software uses numerical techniques to solve models involving fluid flow, heat transfer or mass transfer or a combination of all. The fluid and solid flow and related transport phenomena are governed by a set of partial differential equations (PDE’s), representing the conservation of mass, momentum, thermal energy and chemical species for a fluid or solid element. These governing PDE’s are defined as:

**Continuity equation**

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m
\]  

(8.1)

The continuity equation governs mass conservation. The first term on the left hand side represent the rate of increase of mass in a fluid element, the second represents rate of flow of mass into a fluid element. The right hand term represents the mass added to the continuous phase from the dispersed second phase (e.g., due to vaporization of liquid droplets) and any user-defined sources. For incompressible fluids the density is constant and the first term is zero.

**Momentum equation**

\[
\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = \nabla \cdot (\vec{\tau}) - \nabla p + \rho \vec{g} + \vec{F}
\]

(8.2)

in which the stress tensor \( \vec{\tau} \) is defined as:

\[
\vec{\tau} = \mu \left[ (\nabla \vec{v} + (\nabla \vec{v})^T) - \frac{2}{3} \nabla \cdot \vec{v} \right]
\]

(8.3)

The momentum equation (Navier-Stokes equation) satisfies Newton’s second law; the rate of change of momentum equals the sum of forces acting on an element. The terms refer to:

- \( \frac{\partial}{\partial t} (\rho \vec{v}) \) is the rate of momentum increase of the element
- \( \nabla \cdot (\rho \vec{v} \vec{v}) \) is the net rate of momentum into the element
- \( \nabla \cdot (\vec{\tau}) \) is the surface force on the element due to viscous stress
- \( -\nabla p \) is the surface force on the element due to pressure gradient
- \( \rho \vec{g} + \vec{F} \) is the gravity and other body forces.

**Energy equation**

\[
\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\vec{v} (\rho E + p)) = \nabla \cdot \left( k_{eff} \nabla T - \sum_j h_j \vec{J}_j + (\vec{\tau}_{eff} \cdot \vec{v}) \right) + S_h
\]

(8.4)
In which total energy $E$ is defined as:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2} \quad (8.5)$$

where:

- $k_{eff}$ = effective conductivity,
- $\bar{J}_j$ = diffusion flux of species $j$,
- $S_h$ = heat source,
- $Y_j$ = mass fraction of species $j$ and
- $h_j$ = species enthalpy.

$$h_j = \int_{T_{ref}}^{T} C_{p,j} dT \quad (8.6)$$

$$h_j = \int_{T_{ref}}^{T} C_{p,j} dT \quad (8.7)$$

where sensible enthalpy $h = \sum_j Y_j h_j$ for ideal gases and $h = \sum_j Y_j h_j + \frac{\rho}{\rho}$ for incompressible flows. The energy equation satisfies the first law of thermodynamics; the rate of change of energy equals the sum of the rate of heat addition to and the rate of work done on a fluid element. The term $\frac{\partial}{\partial t} \left( \rho E \right)$ is the rate of increase of enthalpy in a fluid element, the term $\nabla \cdot \left( \bar{v} \left( \rho E + p \right) \right)$ is the convective heat into the fluid element, $\nabla \cdot \left( k_{eff} \nabla T - \sum_j h_j \bar{J}_j + \left( \bar{\tau}_{eff} \cdot \bar{v} \right) \right)$ is the energy transfer due to conduction, species diffusion and viscous dissipation and $S_h$ is the volumetric heat source. In solid regions the equation can be rewritten as seen in Equation 8.8 in which sensible enthalpy $h = \int_{T_{ref}}^{T} C_p dT$.

$$\frac{\partial}{\partial t} \left( \rho h \right) + \nabla \cdot \left( \bar{v} \rho h \right) = \nabla \cdot \left( k \nabla T \right) + S_h \quad (8.8)$$

**Species equation**

$$\frac{\partial}{\partial t} \left( \rho Y_i \right) + \nabla \cdot \left( \rho \bar{v} Y_i \right) = -\nabla \cdot \bar{J}_i + R_i + S_i \quad (8.9)$$

In which the diffusion flux of species $i$, $\bar{J}_i$, can be written as:

$$\bar{J}_i = -\rho D_{i,m} \nabla Y_i \quad (8.10)$$
and for laminar flows

\[ \vec{J}_i = - \left( \rho D_{i,m} + \frac{\mu_i}{S_c} \right) \nabla Y_i \]  

(8.11)

for turbulent flows where

- \( Y_i \) is mass fraction of species \( i \),
- \( D_{i,m} \) is diffusion coefficient for species \( i \),
- \( \mu_i \) is turbulent viscosity and
- \( S_{Ci} \) is the Schmidt number \( \left[ \frac{\mu_i}{\rho D_t} \right] \) where \( D_t \) is turbulent diffusivity.

The species equation describes that the rate of change of the mass of the chemical species per unit volume is equal to the rate of generation of the chemical species minus the convection and diffusion fluxes per unit volume. The first left hand term represents the rate of increase of species \( i \) into the fluid element; the second term the net rate of flow of species \( i \) out of the fluid element due to convection. On the right hand side the first term describes the rate of increase of species \( i \) due to diffusion. \( R_i \) is the net rate of production of species \( i \) by chemical reaction and \( S_i \) is the rate of creation by addition from the dispersed phase plus any user defined sources.

**Equations of state** An extra set of equations is defined to close the system of fluid dynamic equations, it is also necessary to supply relationships between the thermodynamic variables as well as to relate the transport properties to the thermodynamic. The equations used are known as the equations of state, examples of these equations for a perfect gas are:

\[ p = \rho RT, \quad h = C_p T, \quad \sum_{n=1}^{N} C_n = 1 \]  

(8.12)

### 8.3.2 Turbulence models

Turbulent flows are characterised by fluctuating velocity fields. These fluctuations mix transported quantities such as momentum, energy, and species concentration, and cause the transported quantities to fluctuate as well. Since these fluctuations can be of small scale and high frequency, they are too computationally expensive to simulate directly in practical engineering calculations. Instead, the instantaneous (exact) governing equations can be time-averaged, ensemble-averaged, or otherwise manipulated to remove the small scales, resulting in a modified set of equations that are computationally less expensive to solve. However, the modified equations contain additional unknown terms related to fluctuation variables and turbulence models are needed to determine these variables in terms of known quantities.

Amongst other turbulence models, *Fluent 6.1.18* (2003) provides
It is an unfortunate fact that no single turbulence model is universally accepted as being superior for all classes of problems. The choice of turbulence model will depend on considerations such as the physics encompassed in the flow, the established practice for a specific class of problem, the level of accuracy required, the available computational resources, and the amount of time available for the simulation. To make the most appropriate choice of model for your application, the capabilities and limitations of the various options need to be understood. The purpose of this section is to give an overview of issues related to the turbulence models provided in Fluent 6.1.18 (2003), but the Standard k-ε model, the eventual turbulence model utilised in the study, is the only one discussed fully.

**Standard k-ε model** The standard k-ε is a semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate (ε). The transport equations for turbulence kinetic energy and its dissipation rate can be obtained from the Navier-Stokes equations by a sequence of algebraic manipulations. The two equations for k and ε can be expressed as follows:

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k \mu_i) = \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_k}{\sigma_k}) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \tag{8.13}
\]

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon \mu_i) = \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_k}{\sigma_k}) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1\varepsilon} \frac{\varepsilon}{k} (G_k + C_3 \varepsilon G_b) - C_{2\varepsilon} \frac{\varepsilon^2}{k} + S_\varepsilon \tag{8.14}
\]

\(G_k\) represents the generation of turbulence kinetic energy due to the mean velocity gradients and \(G_b\) is the generation of turbulence energy due to buoyancy. \(Y_M\) represents the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate while \(C_{1\varepsilon}, C_{2\varepsilon}\) and \(C_{2\varepsilon}\) are constants. \(\sigma_k\) and \(\sigma_\varepsilon\) are the turbulent Prandtl numbers for \(k\) and \(\varepsilon\) respectively. \(S_k\) and \(S_\varepsilon\) are source terms. The empirical parameters used in this model are listed in Table 8.1.
Table 8.1: Model constants used in the k-\( \epsilon \) model.

<table>
<thead>
<tr>
<th></th>
<th>( C_\mu )</th>
<th>( \sigma_k )</th>
<th>( \sigma_\epsilon )</th>
<th>( C_{\text{sl}} )</th>
<th>( C_{\text{ld}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-( \epsilon ) model</td>
<td>0.09</td>
<td>1.0</td>
<td>1.3</td>
<td>1.44</td>
<td>1.92</td>
</tr>
</tbody>
</table>

The RNG k-\( \epsilon \) model

The RNG-based k-\( \epsilon \) turbulence model is derived from the instantaneous Navier-Stokes equations, using a mathematical technique called "renormalization group" (RNG) methods. The analytical derivation results in a model with constants different from those in the standard k-\( \epsilon \) model, and additional terms and functions in the transport equations for \( k \) and \( \epsilon \). A more comprehensive description of RNG theory and its application to turbulence can be found in user guide of Fluent 6.1.18 (2003).

Realisable k-\( \epsilon \) model

In addition to the standard and RNG-based k-\( \epsilon \) models described above, Fluent 6.1.18 (2003) also provides the so-called realisable k-\( \epsilon \) model. The term "realisable" means that the model satisfies certain mathematical constraints on the normal stresses, consistent with the physics of turbulent flows.

Spalart-Allmaras model

In turbulence models that employ the Boussinesq approach, the central issue is how the eddy viscosity is computed. The Boussinesq hypothesis is used in the Spalart-Allmaras model and the k-\( \epsilon \) model. The advantage of this approach is the relatively low computational cost associated with the computation of the turbulent viscosity. In the case of the Spalart-Allmaras model, only one additional transport equation (representing turbulent viscosity) is solved. In the case of the k-\( \epsilon \) model, two additional transport equations (for the turbulence kinetic energy, \( k \), and the turbulence dissipation rate, \( \epsilon \)) are solved, and viscosity is computed as a function of \( k \) and \( \epsilon \). The disadvantage of the Boussinesq hypothesis is that it assumes viscosity is an isotropic scalar quantity, which is not strictly true. The model proposed by Spalart and Allmaras solves a transport equation for a quantity that is a modified form of the turbulent kinematic viscosity.

Reynolds stress model (RSM)

The Reynolds stress model involves calculation of the individual Reynolds stresses using differential transport equations. The individual Reynolds stresses are then used to obtain closure of the Reynolds-averaged momentum equation. The exact form of the Reynolds stress transport equations may be derived by taking moments of the exact momentum equation. This is a process wherein the exact momentum equations are multiplied by a fluctuating property, the product then being Reynolds-averaged. Unfortunately, several of the terms in the exact equation are unknown and modeling assumptions are required in order to close the equations.

8.3.3 Radiation models

Fluent 6.1.18 (2003) provides five radiation models which allow you to include radiation, with or without a participating medium, in your heat transfer simulations:
The purpose of this section is to give a brief overview of issues related to the above-mentioned radiation models provided in Fluent 6.1.18 (2003), but the Standard P-1 model, the eventual turbulence model utilised in the study, is the only one discussed fully.

**The Standard P1 model** Radiative heat transfer in non-transparent media is governed by the general Radiative Transfer Equation (RTE) of the radiation intensity of the media, expressed in the differential and integral form:

$$\frac{dI(\vec{r}, s)}{ds} + (a + \sigma_s)I(\vec{r}, s) = an^2 \frac{\sigma T^4}{\pi}$$

$$+ \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, s') : \Phi(\vec{r}, s') d\Omega' \quad (8.15)$$

Equation 8.15 describes how the change of the radiation intensity over a certain path length (left hand term) equals the radiation loss due to gas absorption and scattering (first right hand term), as well as the radiation addition by gas emission (second right hand term) and scattering (third right hand term). Apart from particle-particle radiative effects, the gas radiation in this study is modelled by using the standard P1 model. The P-1 radiation model is based on the expansion of the radiation intensity I into orthogonal series of spherical harmonics. The radiative flux is given by Equation 8.16 where G is the incident radiation and C is the linear-anisotropic phase function coefficient.

$$q_r = \frac{1}{3(a + \sigma_s) - C\sigma_s} \Delta G \quad (8.16)$$

By introducing \( \Gamma \) in Equation 8.17, Equation 8.16 simplifies to Equation 8.18.

$$\Gamma = \frac{1}{3(a + \sigma_s) - C\sigma_s} \quad (8.17)$$

$$q_r = -\Gamma \Delta G \quad (8.18)$$
The transport equation for $G$ is defined in Equation 8.19 where $\sigma$ is the Stefan-Boltzmann constant and $S_G$ is a user-defined radiation source.

$$\Delta(\Gamma \Delta G) - aG + 4a\sigma T^4 = S_G \quad (8.19)$$

Equation 8.19 is solved in order to determine the local radiation intensity. Combining Equations 8.18 and 8.19 gives lead to Equation 8.20 which can then be directly substituted into the energy equation to account for heat sources (or sinks) due to radiation.

$$\Delta q_r = aG + 4a\sigma T^4 \quad (8.20)$$

Included in the P-1 model is the capability for modeling anisotropic scattering. Scattering is modelled by a linear-anisotropic scattering function expressed as:

$$\Phi(s' \cdot s') = 1 + C s' \cdot s' \quad (8.21)$$

where $s'$ is the unit vector in the direction of scattering and $s'$ is the unit vector in the direction of the incident radiation. $C$ is the linear-anisotropic scattering phase function which ranges from -1 to 1. In this study the default zero value is used which defines isotropic scattering (Reuter and Yang, 2000). Multiple simulation showed that more advanced models, like the DTRM model used in determining the effective thermal conductivity value, did not provide any significant improvements.

**Rosseland radiation model** The Rosseland approximation method assumes that the media is optically thick and that radiant energy emitted from other locations in the domain are quickly absorbed and have no influence on the local transport. This implies that the approximation is not valid near walls. In Fluent 6.1.18 (2003), special treatment is applied to wall boundaries to overcome this limitation. Other boundaries are not given any special treatment. This approximation is extremely convenient to use, since it does not solve an additional transport equation.

**Discrete transfer radiation model (DTRM)** The main assumption of the DTRM is that the radiation leaving the surface element in a certain range of solid angles can be approximated by a single ray. For models where the radiation field is expected to be reasonably homogeneous everywhere, the Discrete Transfer method can be used. This method is a mixture of the flux type methods and Monte Carlo with a fixed sampling.
Surface-to-surface (S2S) radiation model  The surface-to-surface radiation model can be used to account for the radiation exchange in an enclosure of gray-diffuse surfaces. The energy exchange between two surfaces depends in part on their size, separation distance, and orientation. These parameters are accounted for by a geometric function called a view factor. The main assumption of the S2S model is that any absorption, emission, or scattering of radiation can be ignored; therefore, only surface-to-surface radiation need be considered for analysis.

Discrete ordinates (DO) radiation model  The discrete ordinates (DO) radiation model solves the radiative transfer equation (RTE) for a finite number of discrete solid angles, each associated with a vector direction fixed in the global Cartesian system (x; y; z). The fineness of the angular discretisation is controlled by you, analogous to choosing the number of rays for the DTRM. Unlike the DTRM, however, the DO model does not perform ray tracing. Instead, the DO model transforms into a transport equation for radiation intensity in the spatial coordinates (x; y; z). The DO model solves for as many transport equations as there are directions. The solution method is identical to that used for the fluid flow and energy equations. The implementation in Fluent 6.1.18 (2003) uses a conservative variant of the discrete ordinates model called the finite-volume scheme and its extension to unstructured meshes.

8.3.4 Packed bed: Porous media model

As mentioned in Section 1.3, the constant volume packed bed graphically depicted in Figure 1.1 consists of pellets (apatite), pebbles (silica) and coke, which are assumed spherical in shape. The particles have an average diameter of 2 cm and the packed bed has a porosity of 37.7% at 298K. This value was experimentally determined from actual feed material. The packed bed was simulated by using the Fluent 6.1.18
8.4 Numerical solution of a CFD problem

(2003) porous media model. The model utilises Ergun’s equation. Ergun’s equation is shown in Equation 8.22:

$$\frac{\Delta p}{L} = \frac{150\mu (1 - \epsilon)^2}{D_p^2 \epsilon^3} \nu_\infty + \frac{1.75\rho (1 - \epsilon)}{D_p \epsilon^3} \nu_\infty^2$$

(8.22)

In the porous media model, resistance to flow is simulated by adding a momentum source term ($S_i$ in Equation 8.23) to the standard fluid flow equations. This source term depends on user-inputs for the permeability (see Equation 8.24) and inertial resistance (see Equation 8.25) values in the packed bed.

$$S_i = -\left(\frac{\mu}{\alpha} \nu_i + C_2 \frac{1}{2} \rho \nu_{mag}^2 \nu_i\right)$$

(8.23)

$$\alpha = \frac{D_p^2 \epsilon^2}{150 (1 - \epsilon)^3} \text{ (Permeability)}$$

(8.24)

$$C_2 = \frac{3.5 (1 - \epsilon)^3}{D_p \epsilon^3} \text{ (Inertial Resistance)}$$

(8.25)

8.4 Numerical solution of a CFD problem

**Numerical schemes in Fluent 6.1.18 (2003)**  
*Fluent 6.1.18 (2003)* can use two numerical methods, segregated and coupled solver, to solve the governing integral equations. Both are control volume based methods that consist of:

- Division of the domain into discrete control volumes using a computational grid
- Integration of the governing PDE’s on the control volumes to construct algebraic equations
- Linearisation of the discretised equations and solution of the resultant linear equation system to yield updated values of the dependent variables

**Segregated solver**  
The segregated solver solves the governing equations sequentially, i.e. segregated from one another. To obtain a converged solution many iterations are necessary, each iteration consists of the steps shown in Figure 8.9 and outlined below:

1. Fluid properties are updated, based on the current solution (for the first iteration initialised values are used)

2. The u, v and w momentum equations are each solved in turn using current values for pressure and face mass fluxes, in order to update the velocity field
3. The velocities obtained in step 2 may not satisfy the continuity equation for the volume, and an equation for a pressure correction is derived from the continuity equation and the linearised momentum equations. This pressure correction equation is then solved to obtain the necessary corrections to the pressure and velocity fields and the face mass fluxes to satisfy continuity. The pressure-velocity coupling is achieved by using the SIMPLE algorithm.

4. The equations for the scalars such as turbulence, energy, species, radiation and user defined are solved using the previously updated values for the other variables.

5. A check for convergence of the equation set is made.

The steps are repeated until the required convergence is reached.

**Coupled solver**  The governing equations for continuity, momentum, energy and species transport are solved simultaneously (i.e. coupled together). Governing equations for additional scalars will be solved sequentially using the procedure described for the segregated solver. The iteration loop is shown in Figure 8.9 and outlined below:

1. Fluid properties are updated, based on the current solution (for the first iteration initialized values are used)

2. The continuity, momentum, energy and species equations are solved simultaneously

3. Equations for additional scalars such as turbulence, radiation or user defined are solved using the previously updated values of the other variables

4. A check for convergence of the equation set is made

The steps are repeated until the required convergence is reached.

**Linearisation: Implicit vs. Explicit**  The discrete non-linear governing equations are linearised to produce a system of equations for the dependent variables in every computational cell. This linear system is solved to obtain an updated flow field solution. The governing equations can be linearised in two ways - implicit and explicit:

- Implicit: The unknown variable in a cell is calculated using a relation which includes existing and unknown values from neighbouring cells. Therefore each unknown appears in multiple equations, and these equations must be solved simultaneously.

- Explicit: Each unknown variable is calculated using a relation that includes only existing values. Therefore each unknown will appear in only one equation and the equations can be solved one at a time.
In the segregated solution method implicit linearisation is used. The segregated approach solves for a single variable field by considering all cells at the same time. It then solves the next variable field, again considering all cells at the same time, and so on. There is no explicit option for the segregated solver. A point implicit (Gauss-Seidel) linear equation solver is used in combination with an algebraic multigrid (AMG) method to solve the system of equations.

In the coupled solution method implicit or segregated linearisation of the governing equations are available. These, however, only refer to the simultaneously solved equations. The additional variables such as turbulence, radiation or a user defined scalar are linearised and solved implicitly using the segregated solving method. The coupled implicit approach solves all variables (v, w, u, p, T) in all cells at the same time. A point implicit (block Gauss-Seidel) linear equation solver is used in combination with the AMG method. The coupled explicit approach solves for all variables (v, w, u, p, T) one cell at a time, using a multi stage (Runge-Kutta) solver and the AMG method.

**Discretisation** To solve the PDE’s, first the flow domain is discretised by generating a large amount of cells or control volumes. Fluent 6.1.18 (2003) then uses a control-volume-based technique (finite volume method, FVM) to discretise the governing PDE’s to algebraic equations that can be solved numerically for each cell. This technique consists of integrating the governing equations about each control volume, giving discrete equations that conserve each quantity on a control-volume basis. Using this technique an integral form for an arbitrary control volume \( V \) becomes:

\[
\int \rho \phi \vec{v} \cdot d\vec{A} = \oint \Gamma_{\phi} \nabla \phi \cdot d\vec{A} + \int_V S_{\phi} dV \tag{8.26}
\]
where:

- $\rho$ is density,
- $\phi$ is a scalar quantity,
- $\vec{V}$ is a velocity vector (in 2D),
- $\vec{A}$ is a surface area factor,
- $\Gamma_\phi$ is the diffusion coefficient for $\phi$,
- $\nabla \phi$ gradient of $\phi$ ($= (\partial \phi / \partial x) \hat{i} + (\partial \phi / \partial y) \hat{j}$ (in 2D) and
- $S_\phi$ source of per unit volume.

Equation 8.26 is applied to each control volume, or cell, in the computational domain. The discretisation on a given cell is:

$$\sum_{f} N_{\text{faces}} \rho_f \vec{v}_f \phi_f \cdot \vec{A}_f = \sum_{f} N_{\text{faces}} \Gamma_\phi (\nabla \phi)_n \cdot \vec{A}_f + S_\phi V$$  \hspace{1cm} (8.27)

where:

- $N_{\text{faces}}$ is the number of faces enclosing cell,
- $\phi_f$ is the value of convected through face $f$,
- $\rho_f \vec{v}_f \phi_f \cdot \vec{A}_f$ is the mass flux through the face,
- $\vec{A}_f$ is the area of face $f$,
- $(\nabla \phi)_n$ is the magnitude of normal to face $f$ and
- $V$ is the cell volume

The equations solved by Fluent 6.1.18 (2003) are similar to Equation 8.27 and can be used for multi-dimensional, unstructured meshes composed of polyhedra.

**First- and second-order upwind** Fluent 6.1.18 (2003) stores discrete values of the scalar at the cell centres. However, face values are required in Equation 8.27. These values therefore have to be extrapolated from the values stored at the cell centres. This can be done using an upwind scheme; upwinding means that the face value is derived from quantities in the cell upstream relative to the direction of the normal velocity in Equation 8.27. There are several upwind schemes available in Fluent 6.1.18 (2003): first-order upwind, second-order upwind, power law and QUICK. In this thesis work only first- and second-order upwind schemes were used.

When the first-order upwind scheme is used quantities at the cell faces are determined by assuming that the cell centre values of any field variable represent a cell average value and hold throughout the entire cell; the face quantities are identical to the cell quantities. The second-order upwind scheme cell face quantities are computed using a multi dimensional linear reconstruction method. Higher order accuracy is obtained at cell faces through a Taylor series expansion of the cell centred solution about the cell centroid. The face value is computed by:
\[
\phi_f = \phi + \nabla \phi \cdot \Delta \vec{s}
\]  
(8.28)

with \( \nabla \phi = \frac{1}{N_{\text{faces}}} \sum_f \tilde{\phi}_f \vec{A} \)

where \( \phi \) and \( \nabla \phi \) are the cell centered value and its gradient in the upstream cell, and \( \Delta \vec{s} \) is the displacement vector from the upstream cell centroid to the face centroid. The gradient is calculated using the divergence theorem. Face values \( \tilde{\phi}_f \) are computed by averaging \( \phi \) from the two adjacent cells.

8.5 Building up a CFD model

In the following paragraphs, a typical CFD modelling procedure is introduced (Zhou, 2005), referring to the case involved in this study. The settings for modelling a phosphorus producing submerged arc furnace in this research was briefly introduced as an example and details can be found in the next chapter.

8.5.1 Problem definition

When a CFD simulation is set up, appropriate problem definition is crucial to obtain meaningful results. Definition of model parameters and assumption of model simplifying must be made. General considerations of problem definition for a CFD simulation include computational domain and domain boundaries, two-dimensional or three-dimensional flow, steady or transient flow, laminar or turbulent flow, single or multi-phase flow, compressible or incompressible flow, isothermal or non-isothermal, buoyant or non-buoyant and reacting or non-reacting flow.

In this research, the computational domain is the submerged arc furnace. The furnace consists of a packed bed zone with gas flowing through it. Above the packed bed zone there is a gas zone and two outlet pipes, while within the packed bed zone there are three inlet, or arc zones that introduces the energy to the system. On top of the packed bed domain, an energy sink is defined as the new, fresh Moeller continuously enters the furnace. Underneath the packed bed zone there are slag and ferrophosphorus zones, while around the packed bed zone there is the lining zone representing the furnace itself. The flow is fully three-dimensional, steady-state, turbulent, single phase, compressible, non-isothermal, buoyant and is created from within the packed bed and not introduced to it.

8.5.2 Geometry and domain settings

In this step, the interested simulation area should be decided and properties for every part of it should be defined, e.g. setting up the domains (a fluid domain or a solid domain), setting the domain interfaces, setting sources in domains, such as heat source (volumetric, surface, or point), momentum source, source of chemical species due to reactions, and setting the rotation speed.
In this research, the packed bed zone was defined as fluid domain where resistance to flow is simulated by adding a momentum source term. The energy source and the mass source, as well as the chemical reaction, heating and melting and new feed energy sinks were all included through a user-developed submodel. The slag and ferrophosphorus zones were defined as conducting, non-flowing liquid domains, while the lining zone was defined as a solid domain. The electrodes and feed chutes were also defined as conducting solids.

### 8.5.3 Boundary conditions and initial conditions

The results of CFD simulations are determined by the boundary conditions. It is thus essential that the user specifies boundary conditions correctly and understands the role they play in the numerical solution algorithm. Boundary conditions must be specified and applied by the user to ensure that the problem to be simulated is physically realistic and well posed. The most common boundary conditions are:

- **Inlet**, mass inflow conditions, e.g. velocity, fluid properties, temperature, mass fraction of different species, radiation conditions, etc.
- **Outlet**, external pressure, radiation conditions, etc.
- **Walls**, temperature/heat flux/heat transfer coefficient, friction, and roughness.

In this research, the arc zones created underneath the electrodes were set as the inlet zones for the energy and the outlet pipes were set as the outlet. On top of the packed bed, the continuous entry of fresh feed is simulated by withdrawing energy from this zone. The mass is created from within the packed bed and therefore not attached to the inlet zone. Heat transfer coefficients were known and applied for the outside wall of the furnace. Initial temperature for the entire furnace was set based on real industrial operation and previous simulation results.

### 8.5.4 Physical models selection

The fluid flow equations normally cannot be solved in their exact governing equations. This is because the exact equations either cannot be solved for practical flows of interest, as is the case with turbulent flow. Thus, simplified physical models are employed. Among these physical models, turbulent mixing is the key process responsible for transport of heat, mass and momentum in the vast majority of fluid flows. Other physical models, such as combustion, radiation, buoyancy, rotation, multiphase and reaction models, may be involved as well. Choosing suitable physical models for a specific case is important.

In this research, the most important involved physical models include: turbulent model (standard $k$-$\epsilon$ model), radiation model (standard P-1 model) and the Porous media model.
8.5 Building up a CFD model

8.5.5 Physical properties

Depending on the flow type, some or all of the following properties should be assessed or calculated from the literature or experiments: viscosity, density, heat capacity, thermal conductivity, electrical conductivity, heat transfer coefficient, absorption and scattering coefficients. If they are highly temperature and composition dependent, proper functions need to be provided. It should also be noted that the physical properties are not always well-defined.

In this research, numerous data were obtained from an industrial plant and applied in the process model, e.g. the properties of the gaseous product, Moeller pellets, slag, ferrophosphorus and lining material. Some properties such as the effective thermal conductivity of the packed bed zone was determined through additional modelling and its influence as model parameter were studied.

8.5.6 Numerical calculation and obtaining the results

The processing discussed in the previous paragraphs can be regarded as pre-processing. The followed procedure is to set up the solver-control parameters and activate the solver. To obtain a result sometimes takes hours, days or more, depending on the complexity of the model, the computational cells defined in the grid and the computing power. It is necessary to choose proper solution techniques and controls in order to obtain a more accurate result, a better converge or less CPU computing time. Normally a commercial CFD software sets default solution techniques, which are proper for most of applications. Sometimes, the software provides alternatives which are more suitable for specific situations. To control the solution process, parameters must be defined (Zhou, 2005):

- Maximum iteration number or maximum computing time
- Residual convergence criteria
- Relaxation parameters
- Output controls and monitor controls
- Algorithms

8.5.7 Post-processing of the results

Post-processing involves the analysis of computational results graphically and analytically. All the commercial CFD packages provide good visualisation tools, as well as some professional third-party post-processors, which allow users to check and browse their results in many different ways. These include visualisation of:

- Domain geometry and grid
- Velocity vectors plots
- Line and shaded contour plots
• 2D and 3D surface plots
• Streamlines and particle tracking
• Various outputs possibilities (to files, to printers), or for some packages

In addition, the alphanumeric output in ASCII format e.g. the XY plot for temperature profiles, gives a lot of possibilities for further analysis statistically. These graphical and statistical results can be further edited in PC graphics and spreadsheet programs for reports and presentations.

8.5.8 Validation

CFD modelling generates a huge amount of results in great detail. However, the validity of the results is always very important. In order to have the predictive ability, the models are normally validated with available measurements for flow, velocity vectors or contours, turbulent kinetic energy, temperature or heat flux measurements in the literature, or one has to arrange the measurements from industrial operation, or set up physical models with measurements and simulate the physical model with CFD. The accuracy of the simulation results is a very relative matter. For engineering purposes, it can be very rough, and macroscopic results are sufficient. For more scientific studies, the accuracy needs to be high. However, for simulation of industrial processes, we do not need very high accuracy which would otherwise be too expensive to obtain, and unnecessary.

In this research, the gaseous product-, slag-, carbon furnace lining, the energy distribution between chemical reaction and heating and melting, the mineralogy obtained during a maintenance shut-down and the $P_2O_5_{(\text{slag})}$ wt% were compared with those of the real case in industry and good agreement was obtained.

8.5.9 User expertise

Although CFD codes offer impressive features and the capability to model flows in and around highly complex geometry, the physical and numerical sub-models embodied or applied by the user are, in many cases, often little removed from the relatively crude techniques developed in the early 1970s. In addition, the codes still require considerable user expertise, physical insight and experience if meaningful results are to be generated. Other than the careful processing of definitions, physical properties, model parameters and controls, user interferences into the model is also very important in some special situations. User sub-models, or sub-routines, needed to be developed.

In this research, the energy introduced to the model through the inlet zones is distributed between heating up and melting of the packed bed material and heat distribution associated with the main reactions (simplified to Equation 1.1) within the packed bed. This distribution, as well as the creation of gaseous product through Equation 1.1, was facilitated through the creation of a user developed sub-model
that incorporates all these phenomena. Owing to the fact that the porous media model of *Fluent 6.1.18* (2003) calculates the thermal conductivity of the packed bed as an average of the thermal conductivity based on the volume fraction of the solid (furnace feed) and of fluid (gaseous product), the radiation heat transfer between the particles in the packed bed is not accounted for. In order to therefore improve the standard porous media model for high temperatures, the two conductivity values for the solid (furnace feed) and of the fluid (gaseous product) were replaced by a single, temperature-dependent effective thermal conductivity value representing actual furnace conditions more accurately. The aim was to have an effective thermal conductivity value to be used in *Fluent 6.1.18* (2003) that incorporated both conductive, as well as particle-particle radiative aspects based on actual process conditions. This was done through the creation of a second user developed sub-model. Details of the user sub-model development and integration is introduced and discussed in Chapter 9.
Chapter 9

CFD process modelling: Model development

Within the submerged arc furnace there is a narrow, gas-solid reduction zone in which a very fast reaction takes place over a small temperature gradient. This was shown through the construction of a CFD model by using precise dimensions and actual material properties. Input- and boundary conditions were obtained from plant data. The general purpose CFD code Fluent 6.1.18 (2003) was used to develop the model but the complexities associated with the production of phosphorus necessitated the development of two user-developed models in addition to the standard physical model. These two sub-models successfully combine equilibrium thermodynamics, reaction kinetics and computational flow dynamic calculations. The model was validated through measurements from thirteen temperature probes embedded in the carbon lining, two gaseous outlet temperature probes, 8-hourly slag samples, temperature measurements of the slag stream and calculated specific power consumption values. Results from the model revealed the (i) above-mentioned reaction zone where conditions are optimum for maximum phosphorus recovery, (ii) low, recirculating gaseous flow velocity areas that cause dust accumulation in the outlet pipes and (iii) a zone in the packed bed of little temperature variation similar to the thermal reserve zone in a blast furnace. Energy distributions corresponded well with literature.
9.1 Introduction

Based on the theory and methodology introduced in the previous chapter, the CFD model development procedure and the model configurations are introduced in this chapter. The assumptions and simplifications, the selection of the physical models and model parameters and the details of the development of user-developed sub-models are introduced and discussed in detail. The general results of the developed CFD model are also discussed and presented in this chapter. The CFD model was constructed by using Gambit 2.0.4 (2003) and simulated with Fluent 6.1.18 (2003). Fluent 6.1.18 (2003) has standard physical models to solve most of the required governing equations. The standard physical models used include the standard k-\( \varepsilon \) turbulence model, the P1 radiation model and for the packed bed, the porous media model that use Ergun’s equation. The complexities associated with the production of phosphorus, however, necessitated the development of process specific models. These user-developed models were coded in C++, coupled to Fluent 6.1.18 (2003) and solved exactly the same way as the above-mentioned standard physical models. These user-developed models are called the (1) Reaction model and the (ii) Particle-particle radiation and effective thermal conductivity model. The heating and melting process, the chemical reactions, the development of mass, the introduction of energy to the furnace and a temperature dependent effective thermal conductivity were simulated with two user-developed sub-models. These models are discussed in-depth in Sections 9.6 and 9.7.

9.2 Furnace operation data utilised for CFD model development

In order to develop a reliable submerged arc furnace CFD model, actual process data from Thermphos International were used. Data from 15 August 2005 until 10 May 2006 were collected, filtered and reconciled (see Chapter 5).

9.2.1 Flowrate ranges, energy inputs and temperatures

The 8-hourly averages were then arranged in order of ascending Total pellet flowrate [ton/8hours], with the five ranges utilised shown in Table 9.1. Out of these ranges five main cases or Scenarios representing the averaged data of that particular range, were developed. It is on these five scenarios and derivatives thereof, that the CFD model development were centered (Scheepers, Adema, Yang and Reuter, 2006).

<table>
<thead>
<tr>
<th>Scenario 1</th>
<th>Scenario 2</th>
<th>Scenario 3</th>
<th>Scenario 4</th>
<th>Scenario 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>F-Pellets flowrate ranges</td>
<td>160-180</td>
<td>180-200</td>
<td>200-220</td>
<td>220-240</td>
</tr>
</tbody>
</table>

In Table 9.2 is a depiction of the averaged values that each of the five Scenarios represent. The pellet, silica gravel and coke flowrates are all average values for the
same period. The corresponding energy inputs (MW) are also averaged over an 8-hour period. The gaseous outlet temperature value (E-Temp) is an 8-hour average value for both outlet pipes. The $P_2O_5(slag)$ value is a single 8-hourly sample.

Table 9.2: Average feed flowrates, power consumption values, gaseous outlet temperatures and $P_2O_5(slag)$ values of the five scenarios shown in Table 9.1.

<table>
<thead>
<tr>
<th>F-Pellets</th>
<th>F-SilicaGravel</th>
<th>F-Coke</th>
<th>MW</th>
<th>E-Temp</th>
<th>$P_2O_5(slag)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ton/8hours]</td>
<td>[ton/8hours]</td>
<td>[ton/8hours]</td>
<td>[MW]</td>
<td>[K]</td>
<td>[wt%]</td>
</tr>
<tr>
<td>Scenario 1</td>
<td>170.9</td>
<td>52.0</td>
<td>27.1</td>
<td>37.90</td>
<td>699</td>
</tr>
<tr>
<td>Scenario 2</td>
<td>189.3</td>
<td>58.0</td>
<td>29.8</td>
<td>41.29</td>
<td>711</td>
</tr>
<tr>
<td>Scenario 3</td>
<td>209.2</td>
<td>61.7</td>
<td>32.1</td>
<td>45.38</td>
<td>728</td>
</tr>
<tr>
<td>Scenario 4</td>
<td>228.6</td>
<td>68.8</td>
<td>35.9</td>
<td>48.46</td>
<td>734</td>
</tr>
<tr>
<td>Scenario 5</td>
<td>247.3</td>
<td>72.9</td>
<td>37.7</td>
<td>50.57</td>
<td>748</td>
</tr>
</tbody>
</table>

From Table 9.2 the energy input (MWh) and flowrate values are used as (some of) the inputs to the CFD model, while the $P_2O_5(slag)$ and the average gaseous product outlet temperature (E-Temp) are used for validation purposes. For all five scenarios in Table 9.2 a C-fix = 0.48 (standard deviation = 0.012) was used.

9.2.2 Electrode operating heights

Table 9.3 shows different average electrode operating heights (E-oh-L, E-oh-M, E-oh-R) for each individual scenarios from Table 9.2. These values are average values over an 8-hour period.

Table 9.3: Different electrode operating heights used for the five main scenarios.

<table>
<thead>
<tr>
<th>E-oh-L</th>
<th>E-oh-M</th>
<th>E-oh-R</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scenario 1</td>
<td>68.8</td>
<td>71.4</td>
</tr>
<tr>
<td>Scenario 2</td>
<td>69.5</td>
<td>70.5</td>
</tr>
<tr>
<td>Scenario 3</td>
<td>71.7</td>
<td>74.3</td>
</tr>
<tr>
<td>Scenario 4</td>
<td>67.6</td>
<td>72.9</td>
</tr>
<tr>
<td>Scenario 5</td>
<td>70.3</td>
<td>74.0</td>
</tr>
</tbody>
</table>

9.2.3 Chemical composition

The averaged, chemical analysis values of the input streams of all scenarios are shown in Table 9.4. In order to be used in Factsage 5.4.1 (2006), these values were reworked and grouped (the Moeller feedstream) into actual compounds fed to the furnace e.g. fluoroapatite ($Ca_{10}(PO_4)_6F_2$) and can be seen in Table 9.8 and Appendix E. These values were used throughout this study and only changed in Section 10.3.6.

9.2.4 The Base Case scenario - Scenario 30

Of the above-mentioned scenarios, it is Scenario 3 that best represent the average, steady-state conditions at Thermphos International during the ≈ 6 months under
Table 9.4: The relative concentration of the feed material to the furnace and subsequently to the furnace model. These are concentrations as obtained through XRF analysis and do not reflect the mineralogy inside the feed.

<table>
<thead>
<tr>
<th>Compound</th>
<th>Pellets</th>
<th>Silica Gravel</th>
<th>Coke</th>
</tr>
</thead>
<tbody>
<tr>
<td>P₂O₅</td>
<td>29.1%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>C</td>
<td>-</td>
<td>-</td>
<td>90%</td>
</tr>
<tr>
<td>CaO</td>
<td>45.5%</td>
<td>4%</td>
<td>-</td>
</tr>
<tr>
<td>SiO₂</td>
<td>13.2%</td>
<td>95.0%</td>
<td>8%</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>0.6%</td>
<td>-</td>
<td>2%</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>1.8%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>MgO</td>
<td>0.8%</td>
<td>1%</td>
<td>-</td>
</tr>
<tr>
<td>K₂O</td>
<td>0.3%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Na₂O</td>
<td>0.9%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.4%</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Other</td>
<td>7.4%</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

investigation. However, owing to the fact that this chapter is devoted to a symmetrical base case scenario, all three electrodes were placed at an operating height of 65cm. Scenario 3 with electrodes at equal height is called the Base Case scenario and in Appendix E the base case scenario is numbered as Scenario 30. The base case scenario was used for all CFD model development and subsequent results in this chapter. See Appendix E for the full list of scenario numbers and corresponding data as well as the various electrode operating height variations. The structure where electrode operating heights for all three electrodes are equal at 65cm, is called the E1 structure. It is in Chapter 10 that the other scenarios, as well as their derivatives designed to investigate the sensitivity of certain key parameters, are utilised.

9.3 Furnace dimensions, structure and computational grid

The furnace model to be used in Fluent 6.1.18 (2003) was constructed and meshed in Gambit 2.04 (2003) using the exact dimensions as seen in Figure 9.1. A hexagonal mesh scheme (Cooper type) was used for the furnace and both a tetrahedral/hybrid mesh scheme (T-grid type) and hexagonal mesh scheme were used for the outlet ducts. The total number of cells for the base case scenario is 414000 and typical solving times were between 12 - 20 hours. A cut-through figure of the 3-D constructed furnace can be seen in Figure 9.2, while a section of the computational grid is shown in Figure 9.3.

The entire body of the furnace lining was constructed as a conducting solid using the individual manufacturer specifications of each type of lining. The formation of freezeline was not taken into consideration. The electrodes were modelled with actual property values. Some of these specifications are seen in Table 9.5. The outlet duct has a zero thickness and was abnormally extended in order to establish fully developed flow and at the same time minimise the effect of reversed flow - a phenomenon often encountered in CFD modelling. The packed bed inside the fur-
Furnace is represented with the *Fluent 6.1.18 (2003)* porous media model, as well as with two user-developed sub models. Below the packed bed, the slag and ferrophosphorus phases are simplified as non-flowing, liquid layers but still retain all material properties associated with the respective phases. Although modelling development and results are sometimes presented in a two-dimensional way, this furnace model is entirely three-dimensional and all physical- and user-developed models are solved three-dimensionally.

### 9.4 Furnace body, reactant and product material properties

#### 9.4.1 The body of the furnace

The lining of the furnace consists of carbon bricks in the bottom and lower part of the furnace wall, chamotte bricks in the upper part of the wall and concrete for the furnace lid on top as well as the feed chutes.
Figure 9.2: A graphical representation of the furnace model using Gambit 2.0 (2003) (Adema, 2005).

Figure 9.3: Some of the dimensional grid along with the inlet (arc) zones is displayed. Parts of the furnace structure were deliberately left out in order to depict the inside of the furnace (Adema, 2005).
Chamotte bricks These bricks are made from sintered clay and consist mainly of $\text{SiO}_2$ and $\text{Al}_2\text{O}_3$. *Fluent 6.1.18* (2003) requires the thermal conductivity and density values of the above-mentioned construction material and these specifications were obtained from Thermphos International. Thermal conductivities of the chamotte and the concrete are temperature dependent and the data points, as obtained by the original manufacturers, are shown in Figure 9.4a. Excel was used to construct trendlines which are used in *Fluent 6.1.18* (2003) as material properties. The equation is shown in Table 9.5.

Carbon bricks The specifications given for the carbon bricks from the manufacturer SGL Carbon Group only include the thermal conductivity at 303K which is approximately 7.5 W/mK. However, owing to the high temperatures of the bricks in the furnace a temperature dependent thermal conductivity is highly preferable. Dai and Shu (1999) give a graph with the temperature dependent thermal conductivities of graphite and carbon electrodes which are reproduced in Figure 9.4b. According to the graph, carbon electrodes have a thermal conductivity of 8.3 W/mK at 303K, which is 0.8 W/mK higher than the SGL value. This value was therefore subtracted from all the points of the graph to approximate a temperature dependent thermal conductivity for the SGL carbon bricks. A piecewise polynomial function was determined with trendlines; the thermal conductivity is linear between 273K and 1523K and a polynomial between 1523K and 1773K. Owing to the fact that the graph only has data up to 1773K and temperatures might increase above this value as it is in contact with slag and ferrophosphorus, the conductivity in the last point is taken for all higher temperatures. It would appear that the trendline in the graph rises exponentially and taking the last value would underestimate the conductivity. However, at high temperatures the carbon transforms to graphite and its conductivity starts decreasing.

**Table 9.5:** Physical properties of the concrete top, the chamotte bricks, the carbon lining and pure graphite.

<table>
<thead>
<tr>
<th>Material properties</th>
<th>$k_{\text{cond}}$ [W/m·K]</th>
<th>$\rho$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamotte</td>
<td>$k = 2.31 \cdot 10^{-10}T^3 - 4.76 \cdot 10^{-7}T^2 + 4.85 \cdot 10^{-4}T + 1.04$</td>
<td>$\rho = 2050$</td>
</tr>
<tr>
<td>Concrete</td>
<td>$k = 1.85 \cdot 10^{-4}T + 0.562$</td>
<td>$\rho = 2300$</td>
</tr>
<tr>
<td>Carbon</td>
<td>$k = 0.0017T + 7.041 \quad (273\text{K} - 1540\text{K})$</td>
<td>$\rho = 1570$</td>
</tr>
<tr>
<td></td>
<td>$k = 1.12 \cdot 10^{-4}T^2 - 0.344T + 274 \quad (1540\text{K} - 1773\text{K})$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$k = 15 \quad (&gt;1773\text{K})$</td>
<td></td>
</tr>
<tr>
<td>Electrodes</td>
<td>$k = 23$</td>
<td>$\rho = 1570$</td>
</tr>
</tbody>
</table>

Electrodes The electrodes are manufactured from high quality carbon. The manufacturer specifications provided a thermal conductivity value for the electrode of 23 W/mK at room temperature. No temperature dependent information was included. In Figure 9.4b it can be seen that this is a value between graphite and amorphous carbon. Because the electrode is a nearly immobile solid object extending from the outside into the hottest zone of the furnace a change in thermal conductivity can
have a large influence on the heat distribution and loss. The density of the electrode is 1570kg/m3.

9.4.2 Product material properties

Slag The density of 2964kg/m3 for the slag is calculated using the slag composition from the base case scenario in Section 9.2 and the individual component density data from *HSC Chemistry 5.0* (2002). The literature value for a slag with 55% CaO and 45% SiO₂ was used for the thermal conductivity.

![Thermal conductivities of Chamotte and Concrete.](image)

(a) Thermal conductivities of Chamotte and Concrete.

![Thermal conductivity graphite and amorphous carbon electrodes](image)

(b) Thermal conductivity graphite and amorphous carbon electrodes (Dai and Shu, 1999).

![Slag thermal conductivity](image)

(c) Slag thermal conductivity (*Slag Atlas*, 1995).

**Figure 9.4:** Various thermal conductivity values utilised in the CFD model

The data are shown in Figure 9.4c and a constant value of 0.5 W/mK as determined by Sakuraya was used in preference to Nagata, because their research was focused on high temperatures and is therefore assumed more accurate (*Slag Atlas*, 1995).
The specific heat capacity of the slag was determined at Thermphos International by cooling slag from 1773K to room temperature in water and measuring the temperature rise of the water and was found to be 1260 J/kgK. The value determined by Thermphos International is larger than the HSC Chemistry 5.0 (2002) values for pseudowollastonite and wollastonite (Figure 9.5) at lower temperatures. Owing to the fact that the slag only exists at high temperatures, the Cp used is 1260 J/kgK; the value obtained from Thermphos International which agrees with HSC Chemistry 5.0 (2002) data at higher temperatures.

**Figure 9.5:** Slag specific heat \( (C_p) \).

**Gaseous product** In Fluent 6.1.18 (2003) the temperature dependent density is calculated by the program using the ideal gas law. This was calculated as the volumetric average using heat capacity data from HSC Chemistry 5.0 (2002) for CO(g) and P\(_4\)(g), which is valid for temperatures of 273K up to 6000K. HSC Chemistry 5.0 (2002) gives a piecewise polynomial function for the heat capacity and is simplified by constructing a trendline with Excel seen in Figure 9.6 and shown in Table 9.6. The thermal conductivity of the gas was calculated using theoretical data of CO(g) and P\(_4\)(g) (Yaws, 1995). The temperature ranges do not extend to very high temperatures and the thermal conductivity of the gas is very low compared to that of the solids. For the heat transfer by radiation a continuous value of 0.06 W/mK is chosen for the whole temperature range. This will apply for the gas volume above the packed bed. In the packed bed domain, the gas thermal conductivity will be replaced by an user developed sub-model (see Section 9.8).
Figure 9.6: Product gas specific heat ($C_p$).

Table 9.6: Heat capacity of the gaseous product used by Fluent 6.1.18 (2003) in the gas domain of the model.

<table>
<thead>
<tr>
<th>Gaseous product</th>
<th>Heat capacity, $C_p$ [J/kg·K]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$1 \cdot 10^{-8}T^3 - 9.40 \cdot 10^{-5}T^2 + 0.3 \cdot T + 818$</td>
</tr>
</tbody>
</table>

9.4.3 Reactant material properties

Packed bed  The density and porosity values of the apatite pellets and coke particles were measured by using a mercury intrusion porosimetry technique at the DelftChemTech department of the Delft University of Technology. The technique is based on the principle that mercury is a non-wetting liquid and requires an external force to penetrate voids, the pressure applied can be converted to pore diameter. These results, as well as the specifications for the silica gravel, can be seen in Table 9.7. Given a weight ratio in the Moeller of 68.9% apatite pellets, 10.7% coke and 20.4% silica gravel (see Section 9.2) the Moeller bulk density is $1843 \text{kg/m}^3$. The thermal conductivity of the bed was one of the main challenges of the model. The Fluent 6.1.18 (2003) porous media model calculates the thermal conductivity by taking a volumetric average based on the porosity of the packed bed. Thermal radiation between particles is not taken into account while at high temperatures in the furnace this is a very important way of heat transfer. Two methods were explored in order to determine an effective thermal conductivity value to replace solid and fluid thermal conductivities in the model. The first method culminated in the
development of a user developed sub-model and is discussed completely later.

Table 9.7: The density and porosity values of apatite pellets, coke and gravel.

<table>
<thead>
<tr>
<th>Material</th>
<th>Bulk density $\rho$ [kg/m$^3$]</th>
<th>Porosity %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Apatite pellets</td>
<td>1714</td>
<td>44</td>
</tr>
<tr>
<td>Coke</td>
<td>1230</td>
<td>32</td>
</tr>
<tr>
<td>Silica gravel</td>
<td>2600</td>
<td>-</td>
</tr>
</tbody>
</table>

The second method involved a radiant conductivity model (Singh and Kaviany, 1994). The methods of solving radiative heat transfer in a packed bed can be divided into two types; the medium is considered a continuum or it is considered a discrete collection of particles. The choice of method is based on whether the packing lies in the dependent or independent absorption/scattering range. In the independent scattering range the interaction between radiation and the particle is not influenced by neighbouring particles, the range is limited by a minimum porosity of 95%. Therefore no continuum methods can be used. A discrete particle method to solve the radiant heat transfer in an absorbing, emitting packed bed of spheres was described by Singh and Kaviany (1994). The radiative heat flux for a one-dimensional, plane geometry with emitting particles under steady state conditions is defined by Kaviany (1995).

9.5 Input and Boundary Conditions

There are two energy inputs to the model.

1. Energy Input 1 ($Q_{\text{elec}}$ [Watt/m$^3$]) accounts for the power introduced through the electrodes.

2. Energy Input 2 ($Q_{\text{newfeed}}$ [Watt/m$^3$]) accounts for the new Moeller feed that continuously enters the furnace at a temperature of 573K. Where $Q_{\text{arc}}$ is a positive energy source, $Q_{\text{newfeed}}$ is a negative energy source.

For the graphical depiction of these two energy sources see Figure 9.7.

9.5.1 Energy Input 1: The electrodes

Gu and Irons (1998) employed a channel arc model that showed how the arc from an electrode could be approximated by a cylinder. For this reason, three cylindrical inlet volumes, or zones were created between the electrode tips and the slag surface and the diameter of the electrodes were used as the diameter of the inlet volumes (in Figure 9.3 these inlet volumes are marked as arc zones). The volumes of these zones ($V_{\text{arc}}^1$, $V_{\text{arc}}^2$, $V_{\text{arc}}^3$ [m$^3$]) vary depending on the operating height of the electrodes and provide the model with individual energy input values unique to each electrode. For the base case scenario, each inlet volume is 1.31 m$^3$ in volume. This implies that the point of arc attachment is therefore underneath the electrode. Visual validation of
this assumption was provided when electrode erosion at Thermplos International as a result of arcing was clearly restricted to the bottom of the electrode. Confirmation of this can be seen in Figure 9.8. The power supplied by the three electrode is introduced to the model through these inlet zones (see Equation 9.1). The amount of power introduced to the model in the base case scenario is $Q_{\text{Total}} = 45.38\, \text{MW}$ and the energy input equally distributed over the three arc zones.

$$Q_{\text{elec}} = \left[ \frac{Q_{\text{Total}}}{V_{1\text{arc}}} + \frac{Q_{\text{Total}}}{V_{2\text{arc}}} + \frac{Q_{\text{Total}}}{V_{3\text{arc}}} \right]$$

(9.1)

9.5.2 Energy Input 2: New Moeller feed material

Gravity continuously delivers the new Moeller feed at $\approx 573\, \text{K}$ to the top of the packed bed in the furnace. This is done through ten, evenly distributed feed chutes ensuring constant packed bed volume. This negative energy source ($Q_{\text{newfeed}}$) is employed over the top $0.25\, [\text{m}]$ of the packed bed domain to ensure that the temperature at the top of the packed bed remains at $573\, \text{K}$. Within the coded structure of the model, $Q_{\text{newfeed}}$ is accounted for in the following way:
9.5 Input and Boundary Conditions

Figure 9.8: An actual electrode used at Thermphos International photographed during a scheduled maintenance stop. The electrode erosion is restricted to the bottom of the electrode.

\[
Q_{\text{newfeed}} = \left[ \int_{313K}^{T_{\text{cell}}} C_{\text{pb}} \cdot dT - \int_{313K}^{573K} C_{\text{pb}} \cdot dT \right] \cdot W \cdot \rho_{\text{bulk}} \cdot \frac{1}{z_{\text{cell}}} \quad (9.2)
\]

The heat capacity of the packed bed \( (C_{\text{pb}}) \) was obtained through the generation of a \( Cp \)-graph using Factsage 5.4.1 (2006). It is a function of temperature and Moeller feed composition. This means that every different feed mixture will have a separate \( C_{\text{pb}} \) graph reflecting its own unique heat capacity characteristics. This graph can be seen in Figure 9.12 and will be discussed then.

9.5.3 Energy distribution from literature

In literature, for an industrial phosphorus furnace the energy is distributed between heating up and melting of the material (≈ 40%) and chemical reactions (≈ 45%) (Robiette and Allen, 1972) (Ullmanns Encyclopedia of Industrial Chemistry, 2000). Cooling losses (cooling water), electrical losses (Joule heating) and radiative heat losses account for the additional energy (≈ 15%). The first two energy destinations are discussed later as part of the user developed sub-model section. The additional losses, however, are accounted for in the model by defining accurate boundary conditions. The various boundary conditions are now discussed in Sections 9.5.4 to 9.5.7.
9.5.4 Boundary condition 1 - Bottom and side furnace cooling water

At Thermphos International the outside furnace area adjacent to the carbon bottom area indicated in Figure 1.1 is cooled through a bottom and a side cooling water system which together accounts for \(\approx 3.5\%\) of the total energy consumption. In the model these convective losses were compensated for by introducing averaged, negative heat fluxes [Watt/m\(^2\)] over the bottom cooling, side cooling and electrode cooling surfaces: The bottom cooling losses were set at a constant -1.1MW and the side cooling losses at a constant -0.5MW.

There is no accurate side cooling outlet temperature data at Thermphos International available that allows the effective coupling of e.g. the side cooling flux with the energy input. Moreover, the 13 additionally installed temperature probes have a negligible Pearson correlation with the energy input. The reason for this is the highly dynamic nature of the electrode resistance, and therefore the energy input (power consumption) vs. the time lag between change in the reduction zone, to affect any significant temperature change at the temperature probes that are all 600mm away from the inside of the furnace. For such a temperature change to reach the outside of the furnace where the side cooling water flows down the side of the furnace, takes even longer. It is therefore extremely difficult to give the side cooling-, bottom cooling- and electrode cooling fluxes more accurate values without more accurate measurements. This is not a comment on the Thermphos International measurement practices at all. Even if you had an excessive amount of thermocouples in place, the temperatures will never be able to reflect the extremely dynamic nature of the reduction zone for every ten seconds that the electrode heights are adjusted. It is for this reason that these two negative fluxes were taken as constant for every CFD model in this study.

9.5.5 Boundary condition 2 - Exposed furnace surface

At Thermphos International the stainless steel surface of the furnace exposed to the ambient air (above the wall water-cooled area) has an average surface temperature of \(\approx 373\)K during steady-state operation. This value was determined and validated by actual measurements at Thermphos International. As seen in Figure 1.1 the inside is lined with chamotte bricks that keeps the outside temperature at this relatively low 373K. The average radiative heat loss over this heavily oxidised stainless steel surface is \(\approx 0.8\%\) of the total energy consumption. In the model, radiative heat losses were compensated for by introducing a mixed regime across the relevant surface that included radiation and convective heat losses. The parameters used in Fluent 6.1.18 (2003) are radiation ambient temperature = 623K, emissivity = 0.8 for oxidised steel (Incropera and De Witt, 1990), convection ambient temperature = 573K and convection coefficient = 10 [Watt/m\(^2\)·K].
9.5.6 Boundary condition 3 - Electrode water cooling

The three electrodes are water-cooled at the top of the furnace where they protrude through the concrete roof and where it was originally thought that ≈ 11% of the total energy consumption is accounted for. This high percentage is, in part, attributed to the dissipation of energy through the electrode as part of the Joule heating. Joule heating or ohmic heating refers to the increase in temperature of a conductor (in this case the electrode) as a result of resistance to an electrical current flowing through it. In the model these convective losses were compensated for by introducing averaged, negative heat fluxes [Watt/m²] over the top part of the electrodes. A constant, negative flux of -5MW was set on the top of the electrode surfaces and remained unchanged. This value of -5MW was provided by Thermphos International but because there is no real accurate determination of electrode cooling losses at Thermphos International other values were also tested. It later became evident that only 1MW was closer to reality!

9.5.7 Boundary condition 4 - Heating the Moeller from 313 to 573K

At Thermphos International the part of the feed chutes not protruding into the furnace is more than 20 meters in length as it extend upwards. These parts are called the external feed chutes and is shown in Figure 9.9.

**Figure 9.9:** The Moeller is fed to the furnace through feed chutes that does not form part of the CFD domain as defined in Figure 9.2. Yet, the energy input to the furnace is responsible for heat on the Moeller within these feed chutes and must therefore be compensated for.
The average temperature of the Moeller as it is fed to the furnace at the top of the external feed chutes is 313K. By the time the Moeller enters the furnace, the temperature has increased to approximately 573K. However, these feed chutes do not form part of the CFD domain as defined in Figure 9.2. Yet, the energy input to the furnace is responsible for heating up of the Moeller within these feed chutes and must therefore be accounted for. In other words, at Thermphos International heating up of the Moeller in the feed chutes is an internal heat transfer loop within a furnace domain that, for them, extends all the way up to the top of the feed chutes. The CFD model domain must therefore be treated as a quasi-external heat transfer problem in order to ensure that the Moeller temperature, as it enters the furnace, can be safely initialised at 573K so as to reflect reality. At Thermphos International the Moeller in these feed chutes is heated through the following mechanisms:

- The conduction of heat from the top of the packed bed domain (where it is 573K) up through the Moeller inside the internal feed chutes by means of mainly the coke particle.
- The convection and radiation of heat to the outside of the external feed chutes from the heat released by the transformers, busbars, flexible cables and electrodes on top of the furnace lid.
- The conduction of heat through the oxidised stainless steel surface of the furnace lid to the oxidised stainless steel surfaces of the external feed chutes.

This energy is provided by the Energy Input 1 and is calculated for in the following way:

\[ Q_{\text{feedchutes}} = m_{\text{Moeller}} \int_{313K}^{573K} C_{p_{\text{pb}}} \cdot dT \]  
(9.3)

In the model this energy requirement is accounted for by introducing the appropriate negative heat flux over the same area as the electrode cooling water flux. In the base case scenario this amounts to -2.56MW which brings the total negative flux introduced to the top of the electrode to (-5MW) + (-2.56MW) = -7.56MW.

9.6 Physical Models

In this section the physical models applied in the CFD model are summarised, with all the relevant theory and details already discussed in Chapter 8.

9.6.1 Turbulence model

As mentioned in Chapter 8 several turbulence models are supplied in Fluent 6.1.18 (2003). Here only the widely used k-\( \varepsilon \) model was applied, and other advance models were not used. Multiple simulation showed that this model solved the turbulence effectively, with more advanced model not providing any significant improvements.
9.6.2 Radiation model

Radiation contributes greatly to the heat transfer in the packed bed zone but especially in the gas zone. The goal of radiation modelling is to solve the radiation transport equation, to obtain the source term $S$ for the energy equation and the radiative heat flux at the walls among others quantities of interest. The P-1 model was applied in all the calculations. Multiple simulations showed that more advanced models, like the DTRM model used in determining the effective thermal conductivity value in Section 9.8, did not provide any significant improvements.

9.7 User developed sub-model 1: Reaction Model

The energy introduced to the model through the inlet zones is distributed between heating up and melting of the packed bed material and heat distribution associated with the main reactions within the packed bed. This distribution, as well as the development of gaseous product through Equation 9.9, was facilitated through the development of a Reaction model that incorporates all these phenomena. The following is developed and accounted for in the Reaction model:

1. **Mass development** The gaseous product is produced from within the packed bed domain. This is done in the following way:

   - defining a scalar value representing $P_2O_5$ concentration in the packed bed [kg/m$^3$]
   - the formation of a new transport equation that could transport the user-defined scalar throughout the packed bed domain in a downward direction [kg/s]
   - the decrease of the $P_2O_5$ concentration as a result of Equation 9.9 [kg/m$^3$], along with the resulting generation of gaseous products, $P_4$ and CO [kg/m$^3$]

2. **Reaction energy** The energy required for the main chemical reaction [Watt/m$^3$] is compensated for within the packed bed domain and is linked to the mass development.

3. **Heating and Melting energy** The energy required for the heating and melting of the Moeller, as well as the melted slag and ferrophosphorus [Watt/m$^3$] is compensated for within the packed bed domain and is linked to the heat capacity and the flowrate of the Moeller. These attributes of the Reaction Model are now discussed in detail.

The Reaction model represents the heart of the CFD model and each component of the model will now be discussed in detail.
9.7.1 Mass development

Defining a scalar value representing $P_2O_5$ concentration in the packed bed

A user-defined scalar (UDS) representing the concentration of unreduced $P_2O_5$ in the pellets ($P_2O_5^S$) is defined in the model [kg/m$^3$]. An initialisation value for this UDS of 230kg of $P_2O_5$ per cubic meter corresponds to a 29.1 wt% $P_2O_5$ in the pellets and a packed bed porosity of 37.7% as seen in Scenario 30. This initialisation value is a function of the type of apatite ore, the feed composition, bulk density, particle size distribution and individual particle sizes.

Formation of a new transport equation that could transport the user-defined scalar throughout the packed bed domain in a downward direction

The next step is to simulate downward packed bed movement, because within the CFD model the packed bed itself is stationary. In this way, the UDS defined above ($P_2O_5^S$) can be transported down through the furnace bed. In order to make this possible, Fluent 6.1.18 (2003) can solve the transport equation for an arbitrary, UDS in the same way that it solves the transport equation for a scalar such as species mass fraction.

![Diagram of packed bed with molten slag, thin alloy layer and carbon bottom](image)

Figure 9.10: A cut-through, graphical depiction of the $P_2O_5$ mass flowrate as it moves down the packed bed.

Mathematically this can be described as the formation of an additional advection term within the Fluent 6.1.18 (2003) domain. Advection is transport in a fluid where
the fluid is described mathematically for processes as:

- a vector field (\(\vec{\psi}\)) and
- the material transported as a scalar concentration of substance (\(\phi\)), which is present in the fluid.

This advection term in the differential transport equation has the following general form:

\[
\nabla \cdot \vec{\psi}\; \phi 
\]  
(9.4)

where \(\phi\) represents \(P_2O_5\). In the default advection term, \(\vec{\psi}\) is the product of a scalar density (\(\rho\)) and a velocity vector (\(\vec{v}\)):

\[
\vec{\psi}_{\text{default}} = \rho \cdot \vec{v} 
\]  
(9.5)

where the velocity vector can be specified in three dimensions. In Fluent 6.1.18 (2003) they are defined with the letters U, V or W. Owing to the packed bed moving in a downward direction (radial movement is assumed negligible), W has been defined as the downward velocity of this advection term, in other words the rate of descent of the actual packed bed at Thermphos International (see Figure F.1)! For Scenario 30 the downward velocity term \(W = -1.538e^{-4}\;[\text{m/s}]\).

In order for Fluent 6.1.18 (2003) to properly define and utilise the advection term in Equation 9.4, a special function structure called DEFINE_UDS_FLUX needed to be activated and then re-programmed to facilitate the specific needs this process required. This re-programmed, user-defined function (UDF) can be seen in Figure F.6. For Fluent 6.1.18 (2003) to effectively solve the newly defined transport equation, DEFINE_UDS_FLUX must return \(\vec{\psi}\) back to main Fluent 6.1.18 (2003) program. For this CFD model, the default value (\(\vec{\psi}_{\text{default}}\)) seen in Equation 9.5 was first re-defined as

\[
\vec{\psi} = \vec{v} \cdot \tilde{A} \cdot \rho 
\]  
(9.6)

where \(\tilde{A}\) is the face normal vector of the face of every control volume inside the packed bed. The \(\vec{\psi}\) was then further refined to:

\[
\vec{\psi} = \vec{v} \cdot \tilde{A} 
\]  
(9.7)

where \(\rho\) was removed from the equation. In the UDF this is done by making the value = 1 and is clearly marked in Figure F.1. This means that the value returned to the main Fluent 6.1.18 (2003) program has units of \([\text{m}^3/\text{s}]\). A final look at Equation 9.4 would now reveal a \(P_2O_5\) mass flowrate \([P_2O_5]\) with units of \([\text{kg/s}]\) as it moves down the furnace domain at the speed of the bed packed.

At temperatures \(\geq 1700\text{K}\) (after Wöhler reaction and at pellet collapse) it is likely that the packed bed is made up of mostly solid coke (even extending as far down
as the furnace floor) with slag dripping through it. In order to account for the gas formation and subsequent decrease in packed bed mass flowrate, the value of $W$ is multiplied by a value typically between 0.64 and 0.70. This value is referred to as the flowrate decrease factor (FDF) and is obtained from Equation 9.8. FDF is embedded within the coded structure of the model and can be seen in Figure F.1.

$$\text{FDF} = \left[ \frac{m_{\text{Slag}} + m_{\text{Ferro}} + m_{\text{UnrCoke}}}{m_{\text{Moeller}}} \right]$$ (9.8)

For the calculation in Equation 9.8, it is assumed that the coke bed has the same porosity as the Moeller feed.

**Reaction kinetics, $P_2O_5$ consumption and gaseous product development**

Throughout the iterative solving process of the model, the unreduced $P_2O_5$ left in the pellets ($P_2O_5^{\text{S}}$) is used to calculate the rate of change of $P_2O_5$ concentration in the packed bed ($\Delta P_2O_5^{\text{S}}$) as the reaction takes place. For these calculations Equation 9.9 was used.

$$2Ca_3(PO_4)_2 + 10C + 6SiO_2 \rightarrow P_4(g) + 6[(CaO \cdot SiO_2)] + 10CO(g)$$ (9.9)

The onset temperature of $\approx 1423K$ for $P_2O_5$ reduction was determined experimentally and the reaction is also assumed to take place in two specific steps (Dresen et al., 2002):

$$Ca_3(PO_4)_2 + 3SiO_2 \rightarrow 3[(CaO \cdot SiO_2)] + P_2O_5(g)$$ (9.10)

**Step 1: Liberation**

$$2P_2O_5(g) + 10C \rightarrow P_4(g) + 10CO(g)$$ (9.11)

**Step 2: Diffusion**

Equation 9.9 is a first order reaction, reacting according to a shrinking core model (Mu et al., 1986). In the shrinking core model the $P_2O_5$ gas in Equation 9.10 is liberated from a reaction surface moving from the outside to the inside of the pellet and is controlled by the removal rate of gases from the reaction surface. The reaction constants for a variety of apatite feed ores are calculated from empirical equations obtained experimentally through kinetic investigation of actual feed sample provided by Thermphos International (Van der Pas, 1999). Equation 9.12 shows the experimentally determined reaction constant equation for $X$-type ore, the only one of the investigated type of ores still used at Thermphos International. The use of actual ore highlights the engineering nature of the study.
The rate of change of the P₂O₅ as a result of Equation 9.9 to 9.11 is now calculated through the following derived Equation 9.13, where $t = 1$ second and $k$ the reaction constant of Equation 9.12.

$$\Delta P_2O_5^S = -k \cdot P_2O_5^S(\text{Old}) \cdot e^{-kt} \cdot \left[ \frac{1}{60} \right]$$ \hfill(9.13)$$

The remaining amount of P₂O₅ ($P_2O_5^{S(\text{New})}$) is then given by Equation 9.14.

$$P_2O_5^{S(\text{New})} = P_2O_5^{S(\text{Old})} + \Delta P_2O_5^S$$ \hfill(9.14)$$

Equation 9.15 initialises a new P₂O₅ value for the next iteration (Equation 9.13 once again) in the solving algorithm of the CFD model.

$$P_2O_5^{S(\text{Old})} = P_2O_5^{S(\text{New})}$$ \hfill(9.15)$$

Equations 9.13 to 9.15 are embedded in a coded loop structure within the model.

$\Delta P_2O_5^S$ is the amount of P₂O₅ that reacts according to Equation 9.9. This amount of P₂O₅ decrease in the packed bed is used to determine the volumetric mass generation rate of the gaseous products. From Equation 9.9 it is determined that each kilogram of P₂O₅ produces 0.44 kg of P₄ and 1 kg of CO gas. The amount of P₄ and CO generated is then introduced into the model and the amount of P₄ and CO generated used in the determination of the energy distribution within the packed bed.

**Extra coke addition**  Another aspect to consider is the additional coke fed to the furnace. At Thermphos International this is done (1) to prevent the carbon bricks from reacting, (2) to compensate for the loss of cokes during slag tapping and (3) to compensate the reduction of other oxides like Fe₂O₃ and MnO. Additional reactions involving the extra coke develop an excess amount of gas leaving the furnace that is unconnected to Equation 9.9. This extra gas is introduced artificially to the furnace model at the three inlet volumes underneath the electrodes as described in Section 9.5.1.

**Energy distribution ratio**  It is important to note that the distribution ratio of the input energy in the furnace between the energy required for chemical reactions, as well as the energy for heating and melting is *not* specified when solving the model. These values are essential for validation purposes and generated entirely as dependent variables.
Changing feed mixtures  Heat capacity values in Figure 9.12, and therefore the data in Table 9.8 represent one mixture concentration or recipe of feed material at Thermphos International. By recalculating for a different feed mixture (which will affect Equation 9.12), the influence of changing feed concentrations on the process is investigated. This links well with one of the long term aims of this study - the understanding and eventual minimisation of the varying energy consumption created by complex mixtures of primary and as well as secondary, recycled, phosphorus containing feed materials.

9.7.2 Energy required for the main chemical reaction ($\geq 1423\text{K}$)

For the development of the energy consumption part of the model, chemical reaction and equilibrium software called Factsage 5.4.1 (2006) was used in combination with the official Thermphos International production figures from Aug 2005 until June 2006 [ton/year]. The data were categorised into five classes, using the feed flowrate in descending order. Table 9.8 provides the relative concentration of the feed to the furnace (and therefore to the model). These individual component flowrates were recalculated on the basis of an input of 1kg of P$_2$O$_5$ per second and solved in Factsage 5.4.1 (2006).

![Figure 9.11](image)

Figure 9.11: The energy required for phase transformation, the energy required for subsequent gaseous product and slag formation, as well as the theoretical amount of product (given an initial amount of 1kg P$_2$O$_5$) as calculated by Factsage 5.4.1 (2006).

The equilibrium energy needed as a result of gaseous product formation and phase transformation is calculated as a function of temperature and depicted in Figure...
Table 9.8: The relative concentration of the feed material to the furnace and subsequently to the furnace model. These concentrations are slightly different to the ones provided in Table 9.4 in that it more accurately reflect the mineralogy. This is also the format used as input to Factsage 5.4.1 (2006).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Concentration in feed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca₁₀(PO₄)₆OH₂</td>
<td>25.0%</td>
</tr>
<tr>
<td>Ca₁₀(PO₄)₆F₂</td>
<td>24.4%</td>
</tr>
<tr>
<td>C</td>
<td>10.0%</td>
</tr>
<tr>
<td>SiO₂</td>
<td>28.4%</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>0.6%</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>1.3%</td>
</tr>
<tr>
<td>MgO</td>
<td>0.8%</td>
</tr>
<tr>
<td>K₂O</td>
<td>0.2%</td>
</tr>
<tr>
<td>Na₂O</td>
<td>0.6%</td>
</tr>
<tr>
<td>ZnO</td>
<td>0.3%</td>
</tr>
<tr>
<td>CaO</td>
<td>4.0%</td>
</tr>
<tr>
<td>CaSiO₃</td>
<td>4.3%</td>
</tr>
</tbody>
</table>

9.11 $\left[ \frac{J}{kg \ P_2O_5} \right]$. The twelve values indicated in boldface in Figure 9.11 are used to construct a trendline from which the energy required for gaseous product formation alone at a specific temperature can be obtained. These values are then multiplied with the mass flowrate loss of $P_2O_5$ value within each individual cell contained in the packed bed reactor domain in order to obtain the total energy sink to be employed over the same domain. The calculation is shown in Equation 9.16.

$$Q_R = - (H_R \cdot \Delta P_2O_5^{m}/V_{cell}) \left[ \frac{J}{kg \ s} \cdot \frac{1}{m^3} = \frac{Watt}{m^3} \right]$$

(9.16)

9.7.3 Energy required for phase transformation ($\leq$ 1423K)

Phase transformation below 1423K consumes energy. Figure 9.11 depicts the energy required for this phenomenon as well. It is, however, not possible to connect the overall energy required to the loss of $P_2O_5$ value ($\Delta P_2O_5^{S}$) as was done in the previous section - simply because at temperatures below 1423K the development of gaseous product has not started yet. Therefore, the energy values in Figure 9.11 is employed as an energy sink over each individual cell in the packed bed domain as a function of temperature, total flowrate and cell size.

9.7.4 Energy required for heating and melting of the packed bed

By using data from Table 9.8 combined with Factsage 5.4.1 (2006), heat capacity values for the packed bed ($Cp_{pb}$) were calculated for temperatures between 373K and 3373K. The raw $Cp$ data, as well as corresponding trendlines, are presented in Figure 9.12. In the same figure, four regions of sharp changes in the $Cp$ value are identified in Factsage 5.4.1 (2006). These changes are explained below:

1. Between 1317K and 1318K: $Ca_{10}(PO_4)_6F_2 \rightarrow 3Ca_3(PO_4)_2(whitlockite) + CaF_2$
2. Between 1372K and 1373K: \( \text{Ca}_3(\text{PO}_4)_2(\text{whitlockite}) \rightarrow \text{Ca}_3(\text{PO}_4)_2 \)

3. From 1423K: The main reaction starts taking place and the combined \( \text{Cp} \) of the product and the reactant still increases

4. From \( \approx 1540 \text{K} \): The main reaction proceeds but now the combined \( \text{Cp} \) of the product and the reactant starts decreasing

With temperature dependent \( \text{Cp} \) values available, an energy sink as a result of heating and melting is employed over each individual cell in the packed bed domain through the use of Equation 9.17 within the coded structure of the model. The energy required for heating and melting of the feed is therefore immediately compensated for within each iteration with Equation 9.17 and clearly marked in Appendix F.3.

\[
Q_{HM} = -(\text{Cp}_{pb} \cdot \rho_{\text{bulk}} \cdot \Delta T_{cell} \cdot z \cdot W) \quad \left[ \frac{\text{J}}{\text{kg} \cdot \text{K}} \right] \left[ \frac{\text{kg}}{\text{m}^3} \right] \left[ \frac{\text{K}}{\text{m}} \right] \left[ \frac{\text{m}}{\text{s}} \right] = \text{Watt} \quad \text{(9.17)}
\]
9.8 User developed sub-model 2: Particle-particle radiation and effective thermal conductivity model

Owing to the fact that the porous media model of Fluent 6.1.18 (2003) calculates the thermal conductivity of the packed bed as an average of the thermal conductivity based on the volume fraction of the solid (furnace feed) and of fluid (gaseous product), the radiation heat transfer between the particles in the packed bed is not accounted for. In order to improve the standard porous media model for high temperatures, the two conductivity values for the solid (furnace feed) and the fluid (gaseous product) were replaced by a single, temperature-dependent effective thermal conductivity value representing actual furnace conditions more accurately. The aim was to have an effective thermal conductivity value to be used in Fluent 6.1.18 (2003) that incorporated both conductive, as well as particle-particle radiative aspects based on actual process conditions.

In order to estimate such a thermal conductivity value, a representative volume of the packed bed was constructed by Adema (2005) in Fluent 6.1.18 (2003). This volume was created to be a stripped-down version of the real packed bed that contained pellets (and their corresponding density, thermal conductivity and specific heat capacity values as determined by Thermphos International) as the solid phase and gas consisting of CO and P$_4$ as the gas phase. This volume can be seen in Figure 9.13 and has dimensions of $17.1 \times 5.7 \times 5.7$cm. The stacking of the spheres (pellets) inside the volume has a cubic formation and each of the spheres are 2cm in diameter. The spheres have an overlap of 0.1 cm to simulate compaction and partial melting of the bed, but mainly to improve meshing. The packed bed structure has a porosity of 37%. A t-grid mesh with 470,000 cells was constructed. On the packed bed volume a hot and a cold face with set temperatures were defined. Temperature differences between the two faces were between 288 - 333K, with the eventual average temperatures over the structures seen in Figure 9.13. The remaining boundaries were defined as symmetry faces. No actual gas flow was modelled and the standard porous model was disabled during modelling. The radiation was modelled using the Discrete Transfer Radiation Model (DTRM), which assumes grey radiation and diffuse surfaces and does not include scattering. As the pore spaces are small, the absorption coefficient of the gas was assumed negligible and the solid surface emissivity was assumed equal to 1. The effective thermal conductivity is determined using Equation 9.18, which is based on Fourier’s law of conduction. Fluent 6.1.18 (2003) is used to determine the heat flow ($q$) through the cold and hot faces. The $k_{\text{eff}}$ was determined at different temperatures and with different temperature gradients.

\[
k_{\text{eff}} = q \cdot \frac{L}{A(T_{\text{hot}} - T_{\text{cold}})} \quad (9.18)
\]

The temperature dependent results for $k_{\text{eff}}$ is seen in Figure 9.14, with values for $k_{\text{eff}}$ ranging from 1.15 $[\text{W/m.K}]$ at 373K to 9.21 $[\text{W/m.K}]$ at 2273K. Calculations up to 3273K are possible. The equation in Figure 9.14 was used to generate effective thermal conductivity values that incorporate both conductive, as well as particle-particle
radiative effects. Similar results for grids of 300,000, 500,000 and 1,000,000 cells and volume dimensions of $5.7 \times 5.7 \times 5.7$ cm, $17.1 \times 5.7 \times 5.7$ cm and $28.5 \times 5.7 \times 5.7$ cm confirmed grid and volume independence. Although a particle-particle radiation model is, therefore, not directly available, the effect of such radiation is taken into account by means of the above-mentioned effective thermal radiation value.

**Coke conductivity and Joule heating of the electrodes** In order to compensate for coke conductivity as well as arc radiation, the above-mentioned $k_{\text{eff}}$ was augmented to $2000 \ [\frac{W}{m \cdot K}]$ above $3273K$. The electrode, on the other hand, are subjected to Joule heating during normal operations and to facilitate this in the model, the thermal conductivity value of the electrodes in Table 9.5 was increased from 23 to $4500 \ [\frac{J}{m \cdot K}]$. This also prevented sub-cooling of the top part of the electrode.

### 9.9 Summary of the model configurations

The typical cycle in a submerged arc furnace for the production of phosphorus was considered and simulated as the base case of the process model. In this study the base case scenario is called Scenario 30. The model configurations were summarised as follows, details have been discussed in the previous sections and some parametric studies were carried out for some of the model parameters in the next chapter:

- **Domains:** gas zone, packed bed zone (porous), various lining zones (solid), slag zone (non-flowing liquid), ferrophosphorus zone (non-flowing liquid).
- **Mesh:** a hexagonal mesh scheme (Cooper type) for the furnace, both a tetrahedral/hybrid mesh scheme (T-grid type) and hexagonal mesh scheme for the outlet ducts, the total number of cells: 414 000
9.9 Summary of the model configurations

Figure 9.14: A graph depicting the results of $k_{\text{eff}}$ determined at different temperatures and with different temperature gradients by using Fluent 6.1.18 (2003)

- Steady-state simulation
- Initial temperature of the entire domain: 1700 K.
- Inlet zones: cylindrical areas underneath the electrode for introduction of energy, as well as some small CO as a result of oxide reduction.
- Outlet zones: pressure outlet, gaseous product exit, relative pressure 0 pascal.
- Outer wall surface with water cooling: constant negative heat flux equal to actual conditions
- Outer wall surface above the water cooling: mixed regime cooling with radiation and convection phenomena, environment temperature was set at 350K and the heat transfer coefficient set as $15 \quad \left[ \frac{\text{W}}{\text{m}^2 \cdot \text{K}} \right]$.
- Outer wall surface of the concrete lid: mixed regime cooling with radiation and convection phenomena, environment temperature was set at 400K and the heat transfer coefficient set as $15 \quad \left[ \frac{\text{W}}{\text{m}^2 \cdot \text{K}} \right]$.
- Radiation model: P-1 model with default settings.
- Turbulence model: k-$\epsilon$ model with default settings.
- Two user-developed sub-models: reaction model responsible for the energy distribution between heating up and melting of the packed bed material and heat distribution associated with the main reactions within the packed bed. The effective thermal conductivity model responsible for the incorporation of both conductive, as well as particle-particle radiative aspects in the packed bed based on actual process conditions.
9.10 Base case model results and discussion

In this section the general modelling results are presented for the Base Case scenario (Scenario 30). It demonstrates the capability of the model and the information that can be obtained from its results. It also reveals some important new findings regarding the process. All CFD model results are completely 3D but are presented in a two-dimensional way. Figure 9.15 shows the surface area (marked with the letter C) that is used in most of the graphical presentations.

Figure 9.15: A 2D slice through the right electrode and the right gaseous outlet pipe (Adema, 2005).

9.10.1 Reduction zone and $\text{P}_2\text{O}_5$ consumption

As shown by Dresen et al. (2002) and Van der Pas (1999), optimal reduction of phosphorus takes place in the solid-gas region (packed bed) of the furnace, with the liberated $\text{P}_2\text{O}_5$ gas having to diffuse from the reduction zone inside the pellet, migrate to the coke and then be reduced by the carbon (Dresen et al., 2002). It is, therefore, important to understand the characteristics and behaviour of the gas-solid, main reduction zone within the feed burden where temperatures range from about $1423\,\text{K}$ to about $1723-1773\,\text{K}$. The former temperature refers to the onset of $\text{P}_2\text{O}_5$ liberation, while the latter refers to the temperature where the calcium silicate formation increases to a point where the pellet loses its structure and melts, thereby slowing down the diffusion process. In Figure 9.16 the reduction zone is indicated. It is within the boundaries of this particular area where the main reduction occurs and the gaseous product is optimally generated. For maximum recovery of phosphorus and minimisation of $\text{P}_2\text{O}_5$ wt% in the slag, the reduction zone volume must be as big as possible. In this study, one of the top priorities was the investigation of selected changes in a variety of variables on this reduction zone, as well as the conditions conducive to the maximisation thereof. This will help in understanding and eventual minimisation of the varying energy consumption created by complex feed materials.
9.10 Base case model results and discussion

Figure 9.16: A cross-section of the $P_2O_5$ concentration (UDS) as it is consumed by the reaction. The units on the left are kg of $P_2O_5$ per cubic meter.

Figure 9.16 also shows the decrease in the concentration of $P_2O_5$(pellets) from 29.1 wt% to 2.8 wt% $P_2O_5$(slag). At 1423K the scalar ($P_2O_5$) starts reacting at a value of 230kg of $P_2O_5$ per cubic meter and is virtually depleted by the onset of melting.

9.10.2 Temperature distribution and gaseous product outlet temperatures

Figure 9.17 shows the temperature inside the furnace. The domed-area around the inlet volume (as depicted by the double-sided arrow) depicts the onset of melting. Although not shown here owing to the 1800K upper visual display limit, the average temperature in the inlet volumes (indicated with the thick white and black arrow) is 2700 K. The colder areas indicated with the two ellipses are where cold, fresh feed at a temperature of 573K is artificially introduced to the model - a situation that reflects reality.

9.10.3 Thermal reserve zone

Evidence of a thermal reserve zone like the one found in an iron blast furnace (Peacey and Davenport, 1979) can be seen in Figure 9.18. It shows a plot of packed bed temperature vs. height in the packed bed. The circled area shows rapid cooling and the ellipse an area of less cooling and eventual reaction (where temperature fluctuations are small).
9.10.4 Gaseous product formation and pressure drop in the packed bed

Figures 9.20 and 9.21 show a two-dimensional view of the gaseous product flow vectors from one of the outlet ducts, as well as the velocity contours of both of the outlet ducts. This view provides insight into the causes of high gaseous outlet pressures; low, recirculating gaseous flow velocity areas cause dust accumulation, thus resulting in increased pressure. The furnace under investigation at Thermphos International produced $\approx 3.26 \frac{kg}{s}$ of gas in Scenario 30 and the CFD model flowrate
value of 3.15 [kg/s] (1.58 [kg/s] per pipe) corresponds to within -3.4% of the actual gaseous flowrate. *No constraints are put on this value when solving the model. It is essential for validation purposes and generated entirely as a dependent variable.* Figure 9.19 shows a 45 [Pascal] pressure drop inside the packed bed as calculated by the model.

![Figure 9.19](image1.png)

**Figure 9.19:** A cross-section of the pressure drop inside the packed bed. The unit for the scale on the left is relative pressure in Pascal.

![Average model gas velocity = 4.2 m/s](image2.png)

**Figure 9.20:** Velocity vectors of the gaseous product for one of the outlets. The unit for the scale on the left is m/s.
9.10.5 Energy distribution

In *Ullmanns Encyclopedia of Industrial Chemistry* (2000) it states that for an industrial phosphorus furnace the energy is distributed between heating up and melting of the material (≈ 40%) and chemical reactions (≈ 45%) (Robiette and Allen, 1972) (*Ullmanns Encyclopedia of Industrial Chemistry*, 2000), while cooling losses (cooling water), electrical losses (Joule heating) and radiative heat losses account for the additional energy (≈ 15%). For Scenario 30, the energy input was 45.4 MW and upon convergence the energy output was 46.1 MW. The difference is less than 1.6%. The energy was distributed as follows:

- **40.7%** (18.5 MW) was used for chemical reactions
- **40.1%** (18.2 MW) was used for heating and melting of the material in the packed bed
- **19.2%** (8.7 MW) was contributed to cooling losses that include the gaseous product leaving the furnace.

These values correspond well with the values in the literature. The graphical representations of the results for Scenario 30 are shown in Figures E.1 and E.2, along with a more complete overview of individual contributions of energy consumptions.

**Energy required for the main chemical reaction**  Figure 9.22 shows where the 18.4 MW of energy is extracted from the burden as a result of chemical reactions and the resulting gaseous product formation. The domed area in Figure 9.22 naturally corresponds to the domed area in Figure 9.16 that depicts the consumption of P$_2$O$_5$. 
Figure 9.22: A cross-section of the total energy sink as a result of chemical reactions and the resulting gaseous product formation.

Energy required for phase transformation The energy sink due to phase transformation is located above the reduction zone at a temperature of less than 1423K. It can be seen in Figure 9.23.

Figure 9.23: The energy required for phase transformation.

Energy required for the heating and melting of the packed bed Figure 9.24 shows the places in the packed bed where 18.19MW is extracted as a result of heating and melting. No heating and melting energy are extracted in the reduction zone. These areas are indicated on the figure with two broken arrows.
Further heating (e.g. coke) but mostly melting of additional compounds

Figure 9.24: The energy requirements as a result of heat and melting of the burden.

- Above the reduction zone most of the energy is being used for heating of the Moeller feed, while some slag formation take place.

- Below the reduction zone most of the energy is used for melting as the pellets collapse to form slag together with the silica gravel.

Some of the energy is still used to heat up the coke. The dark section at the top of the packed bed is not shown because it is out of the energy value range of this specific picture. This area depicts the fresh new Moeller feed entering the furnace where most of the energy exchange between the gaseous product and the Moeller feed takes place. In the top part of Figure 9.25 a graphical depiction of the value of the user-defined, specific heat capacity of the packed bed ($C_{pb}$) in the furnace as a results of Figure 9.12 is shown. The bottom part of Figure 9.25 shows a plot of $C_{pb}$ through the centre of the furnace (similar to Figure 9.18) vs. packed bed height.

9.10.6 The $P_2O_5$ content in the slag

In the data range that Scenario 30 represent, the slag stream had a $P_2O_5(slag)$ value = 1.6%. The CFD model generated a $P_2O_5(slag)$ of 2.8%. The $P_2O_5(slag)$ is not directly calculated by Fluent 6.1.18 (2003) but requires additional surface integrations by Fluent 6.1.18 (2003) on the interface between the packed bed zone and the slag zone. This interface, as well as the $P_2O_5$ that reach this interface, is shown in Figure 9.26.
9.11 Model validation

The following measurements at Thermphos International were used to compare with model values and validate the results:

- The temperatures from eight probes radially installed in Furnace 1 at a height corresponding to the reductive zone. These eight probes were installed inside the carbon lining (see Section 3.2.7). Figure 9.27 shows the radial temperature gradient inside the carbon lining at a height of 1650 mm from the bottom of the furnace. The average temperature value of this particular probe (indicated with an arrow) calculated over a period of two months (September and October 2004, as seen in Figure 3.6) was 585K (±61 K). This corresponded well with the model temperature of 660K in the indicated cell.
Figure 9.26: A side and top view of the P$_2$O$_5$ that reach the slag interface. The values on the left of the figures are the scalar values, P$_2$O$_5^S$.

- **The temperatures from five probes vertically installed in Furnace 1.** Figure 9.28 depicts the temperature differences in the top and bottom, vertically-installed, temperatures probes in the chamotte lining adjacent to the packed bed domain. A temperature gradient of 30 °C corresponded well with the average gradient value of 70 °C at Thermphos International during 2005 (Standard deviation on Thermphos International value = ±35 °C).

- **The two on-line, gaseous outlet temperature values from Furnace 1.** The position of the temperature probe in the gaseous outlet pipe at Thermphos International is also shown Figure 9.28. The CFD model temperature of 832K differs somewhat from the 728K shown in bold in Table 9.2, but still falls within the limits of the ±126K standard deviation value of the actual temperature measurement.
• The $P_2O_5_{(slag)}$ values obtained from the laboratory. The actual $P_2O_5_{(slag)}$ for Scenario 30 was 1.6 wt% compared to the 2.8 wt% of the model. The CFD model is 75% higher than the actual but given
  
  – the small amounts of $P_2O_5$ in the slag,
  
  – the 16% standard deviation of $P_2O_5_{(slag)}$ in the Thermphos International slag samples (see Section 3.5) and
  
  – the fact that successive interpolations can lead to small errors in the surface integration report (Fluent 6.1.18 (2003) manual),

this result is not as weak as first would appear. In fact, when later comparing the difference between the actual $P_2O_5_{(slag)}$ vs. the CFD $P_2O_5_{(slag)}$ values in Section 10.2, a strong correlation is found. This validates the ability of the model to simulate even such sensitive parameters, especially with the $P_2O_5_{(slag)}$ being one of the indications of conditions within the furnace.

• The SPC values calculated by Thermphos International. The most important parameter at Thermphos International is the SPC and provides a no-nonsense assessment of the efficiency of the process.

  – In the data range that represent Scenario 30, Thermphos International achieved a SPC of $14.3 \frac{MW\cdot h}{ton\cdot P}$ for Furnace 1.
  
  – The CFD model generated a SPC of $15.3 \frac{MW\cdot h}{ton\cdot P}$.
Figure 9.28: A cross-section of the temperature of the furnace depicting the vertically-installed temperatures probes in the chamotte lining adjacent to the packed bed domain.

This amounts to an absolute difference between the two values of 6.9%. Owing to the fact that the CFD model does not calculate the SPC value directly, some additional calculation is required. The energy input is combined with the amount of P\(_4\) generated by using Equation 9.19. No constraints were put on the variables required for the calculation of the SPC while solving the CFD model. This leaves the solved model SPC values as important validating tools.

\[
\text{SPC} = \left[ \frac{Q_{\text{Total}}}{3.6 \cdot 1000} \right] \cdot \left[ \frac{1000}{\text{mp}_4} \right]
\]  
(9.19)

- The slag temperature of Furnace 1 measured with a pyrometer. An average slag temperature at Thermphos International was measured \(\approx 1750\) K. The temperature of the slag in Scenario 30, CFD modelling results is 1813 K. Considering that the slag temperature at Thermphos International is only measured once a day with a pyrometer, the exact accuracy of the actual value can vary.

- Distributions of energy as put forward by literature sources. The comparison between Scenario 30 results and literature sources like Ullmanns Encyclopedia of Industrial Chemistry (2000) are given in Table 9.9.

Complete result-sheets of Scenario 30 are found in Appendix E.
9.12 Conclusions

This section summarises the first set of conclusions regarding the Scenario 30 CFD model. More detailed conclusions regarding the influence of various key input variables are found in Chapter 10.

- $P_2O_5$ consumption results in Figure 9.16 reveal a narrow gas-solid, reaction zone where conditions are optimum for maximum phosphorus recovery. By identifying the significant operational variables and, more importantly, the influence of changes to these variables on this reaction zone, more knowledge is acquired as to how the furnace can be controlled with the goal of maximising this volume and minimising the energy consumption.

- Gaseous product and velocity information shows low, recirculating gaseous flow velocity areas that cause dust accumulation. This results in increased pressure measurements in the outlet duct.

- The results reveal a zone in the packed bed of little temperature variation similar to the thermal reserve zone in a blast furnace. A reason for this is that most of the heat exchange between the product gas and the Moeller takes place in the top $\approx 40$ cm of the packed bed.

- Energy distributions correspond well with literature.

Table 9.9: The comparison of energy distribution values between Scenario 30 and literature sources.

<table>
<thead>
<tr>
<th></th>
<th>Literature</th>
<th>Scenario 30</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy: Heating and melting</td>
<td>$\approx 40%$</td>
<td>40.1%</td>
</tr>
<tr>
<td>Energy: Chemical reactions</td>
<td>$\approx 45%$</td>
<td>40.7%</td>
</tr>
<tr>
<td>Energy: Cooling losses</td>
<td>$\approx 15%$</td>
<td>19.2%</td>
</tr>
</tbody>
</table>
Chapter 10

CFD modelling scenarios

This chapter validates what was already shown in Chapter 5; that an increase in Moeller flowrate brings about an increase in $P_2O_5$ content in the slag. However, that same increase in Moeller flowrate brings about a decrease in the specific power consumption. This again highlights that a fully dependent variable yields the most influence on the outcome of the process. An increase in $P_2O_{5(pellets)}$ in the Moeller leads to a decrease in the specific power consumption. However, the notion of acquiring only apatite ore with high $P_2O_{5(pellets)}$ in order to continuously obtain such low SPC values, is at the same time offset by unacceptably high increases of $P_2O_5$ content in the slag. An important result is that a change in reaction rate constants has little influence on model results. As long as apatite-type ore is used, the fast reaction time in combination with the long residence time, negates the influence changing reaction rates will have on the process. The fixed carbon-to-$P_2O_5$ ratio is another variable that has limited influence on the outcome of the model. Changing the electrode operating heights in the model has little effect on the outcome; the electrode heights are automatically adjusted every ten seconds and considering the steady-state nature of the CFD model such a result is expected.
10.1 Introduction

Chapter 9 outlined the development and validation of a CFD model for the submerged arc furnace. For this development phase a base case data set known as Scenario 30 was used. In this chapter the accuracy of this developed model is tested outside the data range stipulated by the base case scenario. A series of sensitivity analyses are performed on various key parameters by solving a total of 37 different process scenarios (see Appendix E.3). The results of these analyses and some key conclusions are presented.

10.2 Comparing CFD vs. actual values for the other four scenarios

In this section the five main scenarios obtained in Section 9.2.1 (that includes the base case scenario) were modelled using the E1 electrode structure are presented. Section 9.2.1 provides a detailed explanation of how these scenarios were obtained but Table 10.1 gives an overview of the process values along with the appropriate scenario numbers. The influence of using the actual electrode structures is investigated in Section 10.3.9.

Table 10.1: Average feed flowrates, power consumption values, gaseous outlet temperatures and P$_2$O$_5$(slag) values of the five scenarios shown in Table 9.1.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Scenario 28</td>
<td>170.9</td>
<td>52.0</td>
<td>27.1</td>
<td>37.90</td>
<td>699</td>
<td>1.33</td>
</tr>
<tr>
<td>Scenario 29</td>
<td>189.3</td>
<td>58</td>
<td>29.8</td>
<td>41.29</td>
<td>711</td>
<td>1.31</td>
</tr>
<tr>
<td>Scenario 30</td>
<td>209.2</td>
<td>61.7</td>
<td>32.1</td>
<td>45.38</td>
<td>728</td>
<td>1.59</td>
</tr>
<tr>
<td>Scenario 31</td>
<td>228.6</td>
<td>68.8</td>
<td>35.9</td>
<td>48.46</td>
<td>734</td>
<td>1.64</td>
</tr>
<tr>
<td>Scenario 32</td>
<td>247.3</td>
<td>72.9</td>
<td>37.7</td>
<td>50.57</td>
<td>748</td>
<td>1.86</td>
</tr>
</tbody>
</table>

These scenarios each represent different operating regimes (from high flowrate to low flowrate) on the plant and will test the CFD model’s ability to extrapolate operating regimes outside the base case data range. From a Thermphos International point of view, two of the most important parameters that need to be predicted are:

- specific power consumption
- P$_2$O$_5$(slag)

The values of these parameters for the five above-mentioned scenarios as generated by the CFD model are shown together with the actual values of these two parameters in Figure 10.1. It shows that small differences exist between the SPC values but that the relative differences remain fairly constant at high flowrates. A reason for the CFD model SPC values being consistently higher than the actual values become clear when combined with the P$_2$O$_5$(slag) results; with the way SPC is calculated (Equation 9.19), increased P$_4$ flowrate in the CFD model (while maintaining the
10.2 Comparing CFD vs. actual values for the other four scenarios

Figure 10.1: The CFD vs. the actual values of the P$_2$O$_5$(slag) and SPC values for Scenarios 28, 29, 30, 31 and 32.

Figure 10.2: The CFD vs. the actual values of the gaseous product flowrates and the gaseous outlet temperatures for Scenarios 28, 29, 30, 31 and 32.

same energy input) will decrease the SPC. With the additional P$_2$O$_5$ lost to the slag (2.8% - 1.6% = 1.2% for Scenario 30), a corresponding amount of P$_4$ is not being
produced in the model! This is reflected in the model’s slight under-prediction of the gaseous product flowrate. This is seen in Figure 10.2 that shows the CFD vs. the actual values of the gaseous product flowrates. Even though there is a difference between the two data sets, this difference remains fairly constant. These results show that the model can be used to model regimes outside the data of Scenario 30.

Figure 10.2 also shows the CFD gaseous product temperatures. Considering the large standard deviation values associated with the actual temperature measurements, these predicted values are reasonable. While it is clear that increased Moeller throughput increases the actual temperature, the CFD temperature decreases. The reason for this diverging trend is not quite clear and remains a point for further development.

10.3 Sensitivity analyses of important process parameters

In this section a series of sensitivity analyses are performed on key parameters. These parameters are:

- Moeller flowrate (residence time)
- Fixed carbon-to-P₂O₅ ratio (C-fix)
- Effective thermal conductivity as defined by user developed sub-model 2
- Reaction kinetics
- Packed bed porosity
- P₂O₅(pellets) in the Moeller
- Energy transported away from the furnace through the electrode cooling water
- Electrode operating depths

Apart from quantifying the influence of these parameters on SPC and P₂O₅(slag) values, the following output parameters are also shown in various figures:

- the average slag temperature
- the average packed bed temperature
- the gaseous outlet temperature

Some additional results will be listed in tables which include:

- the energy balance difference; the difference in the balance between energy input and output values within the CFD model as a result of numerical convergence errors and criteria
10.3 Sensitivity analyses of important process parameters

- the gaseous product deviation; the difference in the balance between energy input and output values within the CFD model as a result of numerical convergence errors and criteria
- the % of the input energy utilised for chemical reaction
- the % of the input energy utilised for heating and melting

The following must be noted: every CFD model produces two different SPC values and these are shown in e.g. Figure 10.4 (these two values can also be seen in Figure E.1). This difference is the result of numerical convergence errors on the energy balance of the CFD model, the extent of which differs from scenario to scenario. In Table 10.2 for example there exists a 1.6% energy imbalance within Scenario 30, while the predicted gaseous output flowrate is 3.6% lower than the actual value. These inaccuracies result of numerical convergence errors.

10.3.1 Influence of Moeller flowrate (residence time)

Chapter 5 states that the most influential parameter in the final $\text{P}_2\text{O}_5(\text{slag})$ value is the Moeller flowrate, or residence time in the furnace. This section sets out to validate this finding by exploring the Moeller flowrate and its influence on the CFD model by adjusting the energy input while keeping the flowrate from Scenario 30. The following scenarios (seen in Appendix E.3) were created and solved:

![Figure 10.3: A depiction of the influence of varying Moeller flowrate (residence time) on the CFD model temperatures which include the slag-, packed bed- and gaseous temperature values. Scenario 20 represents a high Moeller flowrate and Scenario 21 represents a low Moeller flowrate. These results confirm dynamic modelling results that the Moeller flowrate is one of the most influential variables.](image)
Figure 10.4: A depiction of the influence of varying Moeller flowrate (residence time) on the $P_2O_5$ (slag) and SPC values. Scenario 20 represents a high Moeller flowrate and Scenario 21 represents a low Moeller flowrate. At lower Moeller flowrates it is clear that increased residence time in the furnace causes the removal of more $P_2O_5$ (slag). However, such a result should always be considered together with a decrease in production rate.

- Scenario 20 uses an energy input of 41.29MW, thereby simulating a higher Moeller flowrate (shorter residence time) relative to the energy input.

- Scenario 21 uses an energy input of 48.46MW, thereby simulating a lower Moeller flowrate (higher residence time) relative to the energy input.

In Figure 10.3 the gaseous product-, the slag- and the average packed bed temperatures for all three scenarios are plotted. With a shorter residence time (Scenario 20), there is less energy available for every cubic meter of Moeller that flows through the furnace.

This results in decreases for all three temperatures. There is less time available for a drive towards a thermodynamic-driven state (equilibrium conditions). Shorter residence time (Figure 10.4) also caused the $P_2O_5$ (slag) to increase to 5.6 wt%. With longer residence times (Scenario 21) all trends are reversed. When interpreting the results in this section it should be noted that at Thermphos International, energy input and Moeller flowrate are linked to each other. Therefore, the one cannot be adjusted independently of the other.

10.3.2 Influence of fixed carbon-to-$P_2O_5$ ratio (C-fix)

In Section 5.2.2 and in Section 7.3.4 it is shown that the $P_2O_5$ (slag) values were largely independent of C-fix. This section sets out to validate this finding. It performs a sensitivity analysis by changing the C-fix values, while keeping the energy input and
Table 10.2: The additional results from the influence of Moeller flowrate, or residence time on the model results relative to the base case.

<table>
<thead>
<tr>
<th>Scenario 20</th>
<th>Scenario 30</th>
<th>Scenario 21</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy balance difference</td>
<td>3.3%</td>
<td>1.6%</td>
</tr>
<tr>
<td>Gaseous product deviation</td>
<td>-12.0%</td>
<td>-3.6%</td>
</tr>
<tr>
<td>Reaction energy</td>
<td>39.8%</td>
<td>40.7%</td>
</tr>
<tr>
<td>Heating and melting energy</td>
<td>36.7%</td>
<td>35.8%</td>
</tr>
</tbody>
</table>

Moeller flowrates exactly the same. The following scenarios (seen in Appendix E.3) were created and solved:

![Graph showing temperature values for packed bed, slag, and gaseous product across different scenarios.](image)

**Figure 10.5:** A depiction of the influence of varying C-fix ratios on the slag-, packed bed- and gaseous temperature values. Result plots from Scenarios 6 (C-fix = 0.43), 7 (C-fix = 0.45), 30 (C-fix = 0.48) and 8 (C-fix = 0.51) confirm that changing C-fix ratios have less influence than changing residence time.

- Scenario 6 uses a C-fix = 0.43
- Scenario 7 uses a C-fix = 0.45
- Scenario 8 uses a C-fix = 0.51

Although the conductivity (effective thermal conductivity sub-model) of the packed bed will be influenced with a change in the C-fix, this value was kept constant in this section. The differences in the presented scenarios therefore come about through changes in the stoichiometry. This changes the $C_{p,\text{pb}}$-curve seen in Figure 9.12.

In Figure 10.5 the gaseous product-, the slag- and the average packed bed temperatures do not show significant variances. In Figure 10.6 the lowest SPC was
Figure 10.6: A depiction of the influence of varying C-fix ratios on the $P_2O_5$ (slag) and SPC values. Result plots from Scenarios 6 (C-fix = 0.43), 7 (C-fix = 0.45), 30 (C-fix = 0.48) and 8 (C-fix = 0.51) show Scenario 30 to have the lowest $P_2O_5$ (slag).

obtained with Scenario 30 and a C-fix = 0.48. Here it also corresponds with the lowest $P_2O_5$ (slag) value but, as seen in Figure 10.7, this is not always the case. This concludes that changes in C-fix do not greatly influence the process. These CFD results contribute to the previously established notion that (while the Moeller flowrate remains constant) C-fix is not an influential parameter.

Table 10.3: The additional results from the influence of C-fix on the model results relative to the base case.

<table>
<thead>
<tr>
<th>Scenario 6</th>
<th>Scenario 7</th>
<th>Scenario 30</th>
<th>Scenario 8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy balance difference</td>
<td>1.8%</td>
<td>1.9%</td>
<td>1.6%</td>
</tr>
<tr>
<td>Gas product deviation</td>
<td>-5.4%</td>
<td>-5.0%</td>
<td>-3.6%</td>
</tr>
<tr>
<td>Reaction energy</td>
<td>41.3%</td>
<td>41.3%</td>
<td>40.7%</td>
</tr>
<tr>
<td>Heating Melting energy</td>
<td>35.6%</td>
<td>35.7%</td>
<td>35.8%</td>
</tr>
</tbody>
</table>

10.3.3 Influence of effective thermal conductivity

This section performs a sensitivity analysis by changing the effective thermal conductivity value represented by the $k_{eff}$-curve in Figure 9.14. For this purpose, seven new scenarios were created and solved. For all of them the inputs of Scenarios 30 were utilised, with the exception of a multiplicative factor associated with $k_{eff}$. It is the value of this factor that is shown on the x-axis of the accompanying figures.

Figure 10.7 shows the gaseous product-, the slag- and the average packed bed
10.3 Sensitivity analyses of important process parameters

...temperature for all seven scenarios. As the multiplicative factor (and therefore the value of \( k_{\text{eff}} \)) increases, all predicted temperatures decrease. Where the \( k_{\text{eff}} \)-value is at its lowest (0.5\( k_{\text{eff}} \)), the input energy is not distributed to the boundaries of the furnace thus not being transferred to the cold Moeller material. This results in the highest gaseous product-, slag- and the average packed bed temperatures. Only once \( k_{\text{eff}} \) is increased by a multiplicative factor of 10 (10\( k_{\text{eff}} \)) do the gaseous product temperature and \( P_2O_5(\text{slag}) \) value in Figure 10.8 record significant deviations. However, the 9.4% energy balance difference and gas product deviation from Table 10.4 makes the result from this scenario less reliable. Apart from this extreme case, chances to the \( k_{\text{eff}} \) value show relatively small changes to \( P_2O_5(\text{slag}) \) and SPC values.

![Figure 10.7: A depiction of the influence of varying effective thermal conductivity values on the slag-, packed bed- and gaseous temperature values. Result plots from 7 variations of Scenario 30 (with each one a different \( k_{\text{eff}} \) value) show, apart from the last scenario (10\( k_{\text{eff}} \)), relatively small changes to the output temperatures.](image)

However, the above-mentioned results should be seen in the following context:

- The \( k_{\text{eff}} \) value and therefore the CFD model do not incorporate the electrical conductivity of the burden.
- The CFD model assumes a perfectly homogeneous packed burden where contact between coke particles are optimal for thermal heat transfer.
- The CFD model assumes a perfectly mixed burden without any segregation.

Once such aspects are incorporated, the results may vary.
Figure 10.8: A depiction of the influence of varying effective thermal conductivity values on \( \text{P}_2\text{O}_5\text{(slag)} \) and SPC values. Result plots from 7 variations of Scenario 30 (with each one a different \( k_{\text{eff}} \) value) show, apart from the last scenario (10\( k_{\text{eff}} \)), relatively small changes to the \( \text{P}_2\text{O}_5\text{(slag)} \).

Table 10.4: The additional results from the influence of \( k_{\text{eff}} \) on the model results relative to the base case.

<table>
<thead>
<tr>
<th></th>
<th>0.5( k_{\text{eff}} )</th>
<th>0.75( k_{\text{eff}} )</th>
<th>Sc 30</th>
<th>1.25( k_{\text{eff}} )</th>
<th>1.5( k_{\text{eff}} )</th>
<th>3( k_{\text{eff}} )</th>
<th>10( k_{\text{eff}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy balance difference</td>
<td>1.7%</td>
<td>1.4%</td>
<td>1.6%</td>
<td>0.6%</td>
<td>0.7%</td>
<td>1.9%</td>
<td>9.4%</td>
</tr>
<tr>
<td>Gas product deviation</td>
<td>-2.5%</td>
<td>-2.7%</td>
<td>-3.6%</td>
<td>-3.0%</td>
<td>-3.4%</td>
<td>-2.8%</td>
<td>9.4%</td>
</tr>
<tr>
<td>Reaction energy</td>
<td>40.4%</td>
<td>40.3%</td>
<td>40.7%</td>
<td>40.1%</td>
<td>39.9%</td>
<td>40.0%</td>
<td>41.5%</td>
</tr>
<tr>
<td>Heating Melting energy</td>
<td>36.1%</td>
<td>35.9%</td>
<td>35.8%</td>
<td>35.4%</td>
<td>35.8%</td>
<td>36.8%</td>
<td>42.0%</td>
</tr>
</tbody>
</table>

10.3.4 Influence of reaction kinetics

The reaction rate constants of the various types of ore were experimentally determined by Van der Pas (1999) and Dresen et al. (2002). Of the four types of ore investigated, only \( X \) type ore is currently used and its reaction rate constant depicted in Equation 9.12. This section performs a sensitivity analysis by changing this value.

The following scenarios (seen in Figure E.3) were created and solved:

- Scenario 9 has a reaction rate constant \( (k_1) = 0.0003T - 0.39 \) (the highest)
- Scenario 10 has a reaction rate constant \( (k_3) = 0.0003T - 0.40 \)
- Scenario 11 has a reaction rate constant \( (k_4) = 0.0001T - 0.125 \) (the lowest)

Figure 10.9 show these four reaction rate constant curves.
10.3 Sensitivity analyses of important process parameters

Figure 10.9: A graphical depiction of the four reaction rate constants used in Scenarios 9, 3, 10 and 11.

\[ k_1 = 0.0003T - 0.39 \]
\[ k_2 = 0.0003T - 0.40 \]
\[ k_3 = 0.0003T - 0.41 \]
\[ k_4 = 0.0001T - 0.125 \]

Figure 10.10: A depiction of the influence of varying ore reaction rates on the slag-, packed bed- and gaseous temperature values, with Scenario 9 having the highest reaction rate and Scenario 11 having the lowest reaction rate. Changes in reaction rates have little influence on these output parameters.

In Figure 10.10 the gaseous product-, the slag- and the average packed bed temperature for all four scenarios indicate very little variation, while the $\text{P}_2\text{O}_5(\text{slag})$
in Figure 10.11 for Scenarios 9, 30 and 10 also remain reasonably constant. The reason for this is the short time required for reduction (Dresen et al. (2002), Van der Pas (1999) and Ershov and Pimenov (1996)) when compared to the 8-12hours residence time of the Moeller in the furnace. Even with the reaction rate increased (Scenario 9) or decreased (Scenario 10), time for reduction is more than enough considering the long time it takes for the burden to reach the slag zone. Also bear in mind that the starting temperature for Equation 2.3 of 1423K (the temperature where the equation’s equilibrium constant ≥ 1) is mostly independent of reaction kinetics. This means that the point where the reactions for the scenarios start, will always start at the same heights within the packed bed. However, the thickness of the reduction zone will change. Therefore, if the reaction rate gets slowed down excessively - as is the case with Scenario 11 - the bottom end of the reduction zone touches the slag interface more and the $P_2O_5$ starts increasing.

However, at high reaction rates melt formation on a micro-scale can block the porous channels of a pellet, thus preventing $P_2O_5$ gas molecule to diffuse to the carbon and thus decreasing the reduction rate (see Section 9.7.1). This is not considered in the model.

**Figure 10.11:** A depiction of the influence of varying ore reaction rate values on $P_2O_5$ and SPC values. It is only at very low reaction rates, as is the case with Scenario 11, that the increased thickness of the reduction zone causes the bottom end of this zone to touch the slag interface. This results in increased $P_2O_5$.

**10.3.5 Influence of porosity**

The aim in this section was to vary only the average packed bed porosity (not individual constituents) and simulate changes in particle sizes of the average pellet, silica gravel or coke particle. This would change the overall porosity of the bed. The
10.3 Sensitivity analyses of important process parameters

Table 10.5: The additional results from the influence of reaction kinetics on the model results.

<table>
<thead>
<tr>
<th></th>
<th>Scenario 9</th>
<th>Scenario 30</th>
<th>Scenario 10</th>
<th>Scenario 11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy balance difference</td>
<td>1.1%</td>
<td>1.6%</td>
<td>2.3%</td>
<td>3.2%</td>
</tr>
<tr>
<td>Gas product deviation</td>
<td>-2.9%</td>
<td>-3.6%</td>
<td>-4.1%</td>
<td>-9.9%</td>
</tr>
<tr>
<td>Reaction energy</td>
<td>40.2%</td>
<td>40.7%</td>
<td>41.7%</td>
<td>43.2%</td>
</tr>
<tr>
<td>Heating Melting energy</td>
<td>35.8%</td>
<td>35.8%</td>
<td>35.6%</td>
<td>35.2%</td>
</tr>
</tbody>
</table>

Porosity of the packed bed was experimentally determined as 37.7 wt% at standard temperature and pressure, while the porosity of the individual feed materials were determined by DelftChemTech department of the Delft University of Technology.

Figure 10.12: A depiction of the influence of varying packed bed porosity on the slag-, packed bed- and gaseous temperature values, with Scenario 12 having the lowest porosity of 35% and Scenario 13 having the highest porosity of 39%.

The following scenarios (seen in Appendix E.3) were created and solved:

- Scenario 12 uses a packed bed porosity = 35.0%
- Scenario 13 uses a packed bed porosity = 39.0%
- Scenario 14 uses a packed bed porosity = 37.7% at the top of the bed with a linear decrease to 32% just above the slag layer

In Figure 10.12 the temperatures revealed little variation. The same can be said for the results depicted in Figure 10.13. Within the CFD model, it is mostly the flow of gaseous product through the packed bed (and thus the momentum source term added to specifically deal with the packed bed) that is affected by a change in
porosity. From these results it is clear that a porosity variation of 4% does not wield great influence on the important process output parameters like $P_2O_5$(slag). Table 10.6 shows the additional results.

![Figure 10.13](image.png)

**Figure 10.13:** A depiction of the influence of varying packed bed porosity on $P_2O_5$(slag) and SPC values.

**Table 10.6:** The additional results from the influence of changing porosity on the model results relative to the base case.

<table>
<thead>
<tr>
<th>Scenario number</th>
<th>Energy balance difference</th>
<th>Gas product deviation</th>
<th>Reaction energy</th>
<th>Heating Melting energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>1.6%</td>
<td>-3.0%</td>
<td>40.7%</td>
<td>35.8%</td>
</tr>
<tr>
<td>30</td>
<td>1.6%</td>
<td>-3.6%</td>
<td>40.7%</td>
<td>35.8%</td>
</tr>
<tr>
<td>13</td>
<td>1.8%</td>
<td>-3.2%</td>
<td>41.0%</td>
<td>35.8%</td>
</tr>
<tr>
<td>14</td>
<td>1.5%</td>
<td>-3.3%</td>
<td>40.7%</td>
<td>35.6%</td>
</tr>
</tbody>
</table>

However, there are two reasons why this porosity sensitivity analyses do not entirely capture the authenticity of the actual process:

- In reality, changes in porosity and, more specifically, to individual constituents like coke, can further affect the packed bed characteristics and cause substantial process fluctuations; at Thermphos International at has been demonstrated that particularly coke size distribution strongly influence the process - more than can be assumed purely on the basis of porosity considerations! Actual test results are confidential.

- Another aspect that reflects actual conditions in the packed bed is a non-homogenous porosity - in a downward as well as a radial direction. A decrease in porosity lower down in any packed bed with reasonably porous material
10.3 Sensitivity analyses of important process parameters

is simply a result of increased pressure brought on by the burden material itself. Scenario 14 simulates a porosity that starts at 37.7% and then linearly decreases to 32% at the slag interface. The latter value was chosen to resemble the porosity of a single coke particle as shown in Table 9.7. The SPC values did decrease slightly, but it is believed that the radial porosity distribution will have the biggest influence on the process outcome. Such a phenomenon will cause channeling of gaseous product and can be implemented in the model at a next stage.

10.3.6 Influence of $P_2O_5$ in the Moeller

Section 7.3.4 states that the $P_2O_5$ in the Moeller ($P_2O_5$\text{\textregistered}pellets) is another influential parameter in the prediction of the $P_2O_5$\text{\textregistered}slag. This section attempts to validate this finding by exploring this parameter and its influence on the CFD model. The following scenarios (seen in Appendix E.3) were created and solved:

- Scenario 15 uses a $P_2O_5$\text{\textregistered}pellets = 27.0%
- Scenario 16 uses a $P_2O_5$\text{\textregistered}pellets = 31.0%
- Scenario 17 uses a $P_2O_5$\text{\textregistered}pellets = 33.0%

The $P_2O_5$\text{\textregistered}pellets is adjusted in the following way:

- In Chapter 9, the apatite ore is represented by (1) fluorapatite, (2) hydroxylapatite, (3) burnt lime (CaO) and (4) wollastonite (CaSiO$_3$). The percentage of $P_2O_5$\text{\textregistered}pellets is changed by changing the fraction of these components within the ore.
- All other components within the apatite ore is kept constant.
- The end-slag basicity does change as a result of this analysis.

In Figure 10.14 all temperatures decrease rather sharply as the $P_2O_5$\text{\textregistered}pellets increases.

**Scenario 17** While the energy input remains the same at 45.38MW, a larger portion of that energy is allocated to the reduction of the increased $P_2O_5$\text{\textregistered}pellets to gaseous product. The effect of this is seen in Table 10.7, where a smaller portion of the energy is left to heat the gaseous product, slag and the packed bed. Noticeable is the lower slag temperature of 1445K in Figure 10.14. Figure 10.15 shows a sharp increase in $P_2O_5$\text{\textregistered}slag.

**Scenario 15** The opposite is observed where less energy is used for chemical reactions than in Scenario 30. The larger portion of the remaining energy increases the gaseous product, slag (T = 1504K) and the packed bed temperatures. Possible benefits as a result of low $P_2O_5$\text{\textregistered}slag = 1.3% is offset by an increase in SPC - the result of less gaseous product formation due to less available $P_2O_5$\text{\textregistered}pellets. The following should be noted:
Figure 10.14: A graph showing the influence of varying $P_2O_5$\textsubscript{pellets} in the Moeller on the slag-, packed bed- and gaseous temperature values, with Scenario 15 the lowest value at 27% and Scenario 17 the highest at 33% $P_2O_5$\textsubscript{pellets}. This variable is significantly influential.

Figure 10.15: A depiction of the influence of varying $P_2O_5$\textsubscript{pellets} in the Moeller on $P_2O_5$\textsubscript{slag} and SPC values, with Scenario 15 the lowest value at 27% and Scenario 17 the highest at 33%. These results validate the finding in Section 7.3.4 which states that the $P_2O_5$\textsubscript{pellets} is an influential parameter in the prediction of the $P_2O_5$\textsubscript{slag}.
10.3 Sensitivity analyses of important process parameters

- Scenario 17 has a high -11.4% deviation on the gaseous product flowrate when compared to the mass balance value. Its results are therefore not as trustworthy as the other scenarios.

- The basicity of the Moeller and the basicity of the final slag is different than in Scenario 30.

- In reality, a change in $P_2O_5$ (pellets) could be associated with a change in energy input.

This section seems to confirm that $P_2O_5$ (pellets) in the Moeller has a strong influence on the furnace process. However, this result should be interpreted together with the above-mentioned constraints.

**Table 10.7:** The additional results from the influence of $P_2O_5$ (pellets) on the model results relative to the base case.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>Energy balance difference</th>
<th>Gas product deviation</th>
<th>Reaction energy</th>
<th>Heating Melting energy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scenario 15</td>
<td>0.9%</td>
<td>1.3%</td>
<td>39.0%</td>
<td>36.8%</td>
</tr>
<tr>
<td>Scenario 30</td>
<td>1.6%</td>
<td>-3.6%</td>
<td>40.7%</td>
<td>35.8%</td>
</tr>
<tr>
<td>Scenario 16</td>
<td>2.6%</td>
<td>-7.4%</td>
<td>42.1%</td>
<td>35.4%</td>
</tr>
<tr>
<td>Scenario 17</td>
<td>2.4%</td>
<td>-11.4%</td>
<td>43.1%</td>
<td>34.1%</td>
</tr>
</tbody>
</table>

10.3.7 Influence of electrode water cooling (Boundary condition 3)

Thermphos International revealed that during normal operational conditions, an average of 5MW is lost through the three electrodes by means of the cooling water. This is due, in part, to a large portion of the energy released by the arc being dissipated in the electrode (Guo and Irons, 2005).

In the CFD model, the energy is introduced to the user-developed inlet (arc) zones and no current actually flows through the electrodes. For this reason the thermal conductivity value of the electrodes provided by the manufacturer in Table 9.5 was increased from 23 to 4500 J m$^{-1}$ K$^{-1}$. In this way the required 5MW could be extracted from the furnace model and thus, prevent the sub-cooling of the top part of the electrode grid. It is recognised that such artificial augmentation could have an impact on modelling results. In order to assess its influence, the negative energy sink of -5MW associated with Scenario 28 was decreased to -4.5MW and -4MW respectively, the scenario re-modelled and the results presented below.

In Figure 10.16 the gaseous product-, the slag-, the average packed bed temperature and the exposed electrode surface temperatures just above the packed bed are depicted. The exact location of the measurement for the exposed electrode surface is shown in Figure 10.18a. With the electrode cooling at -4MW, the exposed electrode surface temperature increased by $\approx 100$K. A reason for this is that at -4MW electrode cooling flux, less energy is being withdrawn from the electrode while the
same amount of energy is introduced to the inlet (arc) zones; this increases the exposed electrode surface and subsequently also the gaseous product-, the slag- and the average packed bed temperatures. Results from Figure 10.17 and Table 10.8 show that the increased energy that remain in the furnace, decreases the $P_2O_5$ (slag). This decreases the gaseous product deviation and subsequently lower the SPC.

### 10.3.8 Revised Scenario 30 and the ultimate emphasis on the effect of accurate process data

During the final stage of revision of this study it was revealed that the actual value of the electrode cooling flux shown in Section 9.5.6 was not -5MW but rather the significantly lower value of -1MW. For this reason the electrode cooling flux was adapted and Scenario 30 solved again.

In Figures 10.19 and 10.20, the results of the Revised Scenario 30 were superimposed onto the pictures from Section 10.2. Replacing -5MW with -1MW (while keeping everything else constant) resulted in the following:

- **SPC (revised)** = 14.8 [MWh/ton P₄]
- **$P_2O_5$ (slag) (revised)** = 2.1 %
- **Gaseous product flowrate (revised)** = 3.23 [kg/s]
- **Gaseous product temperature (revised)** = 934 [K]

It was also written in Section 10.2 that with the additional $P_2O_5$ lost to the slag (2.8% - 1.6% = 1.2%) in Scenario 30, a corresponding amount of P₄ is not being produced in the model and that this is reflected in the model’s slight under-prediction.
10.3 Sensitivity analyses of important process parameters

Figure 10.17: A depiction of the influence of changing the cooling flux to the top part of the electrode on $P_2O_5$ (slag) and SPC values.

Figure 10.18: Some CFD modelling results of the gaseous product flowrate. Now, Revised Scenario 30 provided a $P_2O_5$ value of 2.1 % (2.8% - 2.1% = 0.7%) and has therefore resulted in the gaseous product flowrate increasing to 3.23 [kg/s] - very close to the actual value of 3.26 [kg/s]! This, in turn, also led to the decrease in SPC to 14.8 [MWh/ton P₄] - also a lot closer to the actual value of 14.3 [MWh/ton P₄]. The reason for the improved results is the extra 4MW introduced to the furnace. This energy allowed more apatite to react,
One result where the values moved away from the actual value is the gaseous outlet temperature. This could be improved by bolstering heating and melting investigations of the Moeller with the help of *Factsage 5.4.1* (2006) and the newly available databases.

### Table 10.8: The additional results from the influence of changing electrode cooling flux by using Scenario 28.

<table>
<thead>
<tr>
<th></th>
<th>4MW</th>
<th>4.5MW</th>
<th>Scenario 28</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy balance difference</td>
<td>1.8%</td>
<td>2.5%</td>
<td>2.5%</td>
</tr>
<tr>
<td>Gaseous product deviation</td>
<td>-2.5%</td>
<td>-3.2%</td>
<td>-3.3%</td>
</tr>
<tr>
<td>Reaction energy</td>
<td>38.1%</td>
<td>38.2%</td>
<td>38.4%</td>
</tr>
<tr>
<td>Heating and melting energy</td>
<td>36.4%</td>
<td>36.1%</td>
<td>35.7%</td>
</tr>
</tbody>
</table>

### 10.3.9 Influence of the electrode operating depths

Owing to the fact that electrodes could move up and down as a result of changing packed bed thermal conductivity and therefore C-fix, changing electrode operating heights were simulated at C-fix = 0.43 and at C-fix = 0.48.

- The first part looks at extreme electrode operating heights. To investigate this, the E8 and E9 electrode structures as shown in Figure E.5 were used. For C-fix = 0.48, Scenario 23 represent the E8 electrode structure where the middle...
10.3 Sensitivity analyses of important process parameters

Figure 10.20: The CFD vs. the actual values of the gaseous product flowrates and the gaseous outlet temperatures for Scenarios 28, 29, 30, 31, 32 and the Revised Scenario 30 given a 1MW electrode cooling rate.

Figure 10.21: Results generated by changing the operating heights of the electrodes given a C-fix = 0.48. The influence of varying electrode operating heights is small.

electrode operates 20cm above the other two, while Scenario 24 represent the E9 electrode structure where the middle electrode operates 10cm above the left electrode and the left electrode operates 10cm above the right electrode. For C-fix = 0.43, Scenario 35 represent the E1 structure, Scenario 26 the E8 electrode structure and Scenario 27 the E9 electrode structure. In reality, these
operating height differences are seen as extreme. In Figures 10.21 and 10.22 the gaseous product-, the slag- and the average packed bed temperatures for both these C-fix values are shown. The results show very little temperature differences between extreme electrode operating configurations or differing C-fix values.

- In Section 10.2 actual process results were compared with CFD results by using the E1 electrode operating height structure. Here the actual electrode operating heights associated with the three flowrate regimes associated with Scenario’s 29, 30 and 31, were used for comparison. The scenarios used were Scenario 2 (E3 structure), 3 (E4 structure) and 4 (E5 structure) and the results are seen in Figures 10.25 and 10.26. This was done in order to determine if asymmetrical electrode operating heights affected the CFD results. As can be seen from these two figures, changes in the operating heights made little difference in the CFD model results.

It should be re-stated that the operating heights of the electrodes can not be adjusted directly, but change automatically.

10.4 The outlook for the Dynamic-CFD hybrid model

How the dynamic predictive model and the steady-state CFD model could be combined into one representative model was answered in Part II. It presented a conceptual framework for a Dynamic-CFD hybrid model. If the Dynamic-CFD hybrid model combine the two modelling techniques in the way described, could their respective predictive and modelling abilities compliment each other in such a way as to
10.4 The outlook for the Dynamic-CFD hybrid model

Figure 10.23: A depiction of the influence of changing electrode operating heights of the electrodes given a C-fix = 0.48 on $P_2O_5$ (slag) and SPC values. The effects are small.

Figure 10.24: Results generated by changing the operating height of the electrodes given a C-fix = 0.43 and the influence of these changes on $P_2O_5$ (slag) and SPC values.
Figure 10.25: The temperature results of the actual electrode operating heights associated with three flowrate regimes alongside the results from the E1 electrode structure.

Figure 10.26: Apart from the (2 vs. 29) structure, the \( \text{P}_2\text{O}_5(\text{slag}) \) and SPC results show almost no change in value for the different structures.
provide improved overall predictions? There are some intrinsic difficulties associated with such a Dynamic-CFD hybrid model:

**The Thermphos-sampling interval**

This interval is approximately 8 hours. During the 8 hours that no sampling is done, valuable process dynamics and history that will enhance and strengthen the dynamic model’s predictive ability get lost. *Any predictive model is only as good as the data used to develop it!* Further improvement to the dynamic model is, therefore, possible through a decrease in the Thermphos-sampling interval. However, industrial sampling are expensive undertakings involving well-trained staff, expensive equipment and, more often than not, on-site laboratories already understaffed and overbooked. Any decrease in sampling interval would involve increased sampling analysis - an exercise that will always become a cost optimisation problem.

**The model-sampling interval**

This interval is exactly 8 hours and was chosen to reflect reality and to investigate the influence of operator tools on the outcome of the process. Additional model development using *MATLAB* (2007) revealed that decreasing the model-sampling interval to 1 hour by utilising zero-order holds on the flowrate- and composition data sets, decreased the accuracy of the prediction. It was thought that continuously updated electrical data like electrode operating heights would compensate for the under-sampled flowrate- and composition data and improve predictions but this was not the case. Even 1-hour, averaged values proved as ineffective as 8-hour, averaged values. This is because the rates of change in these electrical data are sometimes as frequent as every second. Increasing the model-sampling interval, on the other hand, increased the accuracy of the prediction - if only due to the fact that the influence of residence time diminishes as the model-sampling interval becomes more than 12 hours.

**The steady-state nature of the CFD prediction**

This provides unique challenges. The results it generates are in good agreement with averaged data from the actual process and can provide valuable insight with regards to long-term step changes to input conditions. Examples of these are new and cheaper apatite ore, new and less porous coke, smaller and sieved silica gravel particles etc. However, the model’s predictive effectiveness diminishes when short-term, impulse changes are to be modelled; the kinds of changes that occur every second during the process. These include changing electrode operating heights.

These difficulties do not make implementation of the model impossible but, given the current status quo, make such an exercise less effective. Given the following recommendations, the concept can yet play a more prominent role. This means that, in the absence of decreased Thermphos-sampling intervals, the dynamic model’s prediction ability will decrease when model-sampling intervals are decreased. At the same time the predictions of the CFD model will also become less and less
reliable if it is attempted to model shorter, instantaneous snapshots. Therefore, if the Dynamic-CFD hybrid model is implemented as part of a predictive control loop today, the accuracy could never account for more than 35% of the variance in the P_2O_5(slag). This in no way negates the conceptual framework of the Dynamic-CFD hybrid model, but places it in perspective with the operational costs involved with sampling analyses of a modern-day industrial plant. Little predictive improvement will be possible without upfront expenses.

10.5 Conclusions

The most important result is the identification of a distinctly narrow gas-solid, reduction zone where a very fast reaction takes place over a small temperature gradient. A first attempt was made to quantify the influence changes some significant operational variables would have on this reduction zone. In this way more knowledge is acquired as to how the furnace can be controlled with the goal of maximising this volume and minimising the energy consumption.

The reduction zone Figure 9.16 and Appendix E.14 provide two dimensional and three dimensional pictures of this reduction zone (Scenario 30).

- The upper boundary of this reduction zone is mainly determined by the chemical composition of the pellet, bed conductivity and bed permeability i.e. the major variables controlling conduction and convection phenomena within the bed.

- The lower boundary of this reduction zone (and therefore the thickness thereof) is mainly determined by the structural qualities of the sintered pellet, the porosity of the pellet and, to a lesser extent, the reaction rate kinetics. The liberated P_2O_5(g) must diffuse through the pellets pores and react with the carbon on the coke surface. It is this step that is rate-limiting and not the reaction rate. If, within the reduction zone, the pellets were to mechanically collapse, this diffusion step and the important convection phenomena transporting the energy, would be impeded and the lower boundary would be reached. The same would happen if slag components like SiO_2 and CaO start reacting locally within the pellet, thereby closing the pellet pores.

The sensitivity analysis

- It was established in Part III that Moeller flowrate was the variable with the most influence on the P_2O_5(slag). This conclusion was validated with the CFD model. However, it should again be noted that at Thermphos International, energy input and Moeller flowrate are linked to each other. Therefore, the one can not be adjusted independently of the other.

- It was established in Part III that P_2O_5(pellets) in the Moeller is another variable that has a large influence on the P_2O_5(slag). This conclusion was also validated by the CFD model. However, the following should be taken into account: (1)
localised melting phenomena within individual pellets were not considered and (2) real energy input fluctuations as a result of changing $P_2O_5(\text{pellets})$ values were not explored and form part of future work.

- It was shown in Section 5.2.2 and depicted in Figures 5.2 that C-fix had limited influence on the $P_2O_5(\text{slag})$. This conclusion was validated through the CFD model for C-fix between 0.43 to 0.51. Subsequent alterations to the conductivity as a result of changes in the C-fix (thermal and electrical) were not considered here.

- Incremental changes to the effective thermal conductivity value (while keeping the C-fix constant) had little influence on the $P_2O_5(\text{slag})$ and SPC values. This shows that a furnace with a *perfectly mixed* burden could effectively operate within a substantially large range of $k_{\text{eff}}$ values. Not considered here is sudden changes that an immediate and large increase in C-fix could have on the gaseous product temperatures.

- Changing reaction rates had little influence on the important process parameters. This proved that the time required for theoretically complete reduction is so short when compared to the 8-12 hours residence time, that it can be seen as quasi-steady state. Even with the reaction rate artificially increased or decreased, especially the gaseous product temperature and $P_2O_5(\text{slag})$ remain fairly unchanged. Only when the reaction rate gets slowed down excessively (artificially or naturally), as is the case with Scenario 11, the lower boundary of the reduction zone starts touching the slag interface and increases $P_2O_5(\text{slag})$. This validates the choice not to pursue further reaction kinetic studies (one of the original project objectives of this project) on apatite ore.

- A homogeneous and overall porosity variation of 4% did not have a large influence on the important process parameters. Even a linear porosity change in the downward direction (z) proved to have little effect. Changes to only the coke particle size distribution were not modelled. This could alter the conductivity path, thus influencing the overall process.

- Changing the electrode operating heights in the model had little effect the important process parameters. Considering the steady-state nature of the model, such a result is expected; the automated control adjusts the operating heights of the electrodes almost every second.

**Revised Scenario 30** Process data significantly different from the value used to construct the model (but closer to actual values) was introduced at a very late stage in the project; the model not only absorbed these change, but improved on the results. This showed that the CFD model is robust, non-stiff (in a differential equation sense) and reflects reality very well (within the fundamental limitation). However, the gaseous outlet temperature did worsened by 100K and by using Figure 9.6 and a gaseous flowrate of 3.23 [kg/s], this extra 100K results in an additional 0.32MW of energy that leaves the furnace. It is thought that this energy could be
connected to the heating and melting or the chemical reactions inside the packed bed.

**Additional model assumptions and limitations**  No gas-liquid reactions within the slag were considered and no side-arcing from the electrodes were modelled.
Part V

CONCLUSIONS AND RECOMMENDATIONS
Chapter 11

Conclusions and Recommendations

The study reveals a narrow, gas-solid reduction zone in which a very fast reaction takes place over a small temperature gradient. Above this reduction zone, there exists a region in the packed bed of little temperature variation similar to the thermal reserve zone in a blast furnace. Varying reaction rate kinetics have a limited effect on the important process outputs of the process. Both the CFD model and the dynamic model provide the same prognoses on general process trends and validate the accuracy, as well as the legitimacy of the two modelling methods. However, fundamental design-, sampling- and process restrictions limit the predictive and especially control accuracy or meaningfulness of the dynamic model - prediction is only as good as the data it uses to generate that prediction! For that reason, these restrictions also limit the accuracy of the CFD model. The point is made that, given the current status quo, no dynamic prediction model or CFD model can improve on an 8-hour-ahead prediction of 30% (6%). This barrier can only be pierced with e.g. tidier and more frequent sampling and other upfront capital investments. Only once that is done, the vision for a better CFD model will become attainable. Such a decision become a cost analysis exercise and one that can only be taken at management level. In summary, this thesis has integrated data collected from a digout by the author, used results from extensive sampling of the slag streams and utilised data from feed material porosity tests and thirteen additional temperature probes installed inside the furnace lining. The author subsequently used these data in dynamic as well as CFD models of the furnace to evaluate the value of these models and its value to industry.
11.1 Conclusions

General

- Asymmetrical furnace operation negatively influences the phosphorous production process. Such asymmetrical behaviour largely stems from unequal tapping - the temptation to abandon standard protocol and keep on tapping at the same slag tap hole as long as the slag flows freely. However, simply enforcing a 50/50 slag-tapping policy on an already eroded furnace might decrease productivity.

- There exists a standard deviation of 16% with regard to the $P_{2}O_{5\text{(slag)}}$ in a single slag sample. Therefore, any model using $P_{2}O_{5\text{(slag)}}$ as a variable will always have at least a 16% inherent uncertainty already encapsulated therein.

Data mining and the dynamic model

- The residence time of the feed material (Moeller flowrate) is the overriding and most influential process variable. Unfortunately, it is completely dependent and cannot be controlled directly.

- No significant statistical correlation exist between $P_{2}O_{5\text{(slag)}}$ values and C-fix.

- Cost analysis reveals that a drive for improved specific power consumption should always supersede the drive to decrease the $P_{2}O_{5\text{(slag)}}$.

- The furnace is continuously fluctuating back-and-forth between a dynamic-driven state and a thermodynamic-driven state. It is owing to this fluctuating state in the furnace that linear modelling techniques provide similar predictive abilities than non-linear techniques.

- A linear, adaptive prediction model with an auto-regressive, exogenous input structure (ARX) achieved an 8-hours-ahead predictive accuracy of 30% ($\pm 6\%$) on future $P_{\text{slag}}$ values. This is possible because the long residence time ensures that some metallurgical memory (data history) is always present in the process.

- C-fix and the silica gravel factor are two independent variable used by operators in an attempt to steer the process within given output setpoints. A linear, adaptive predictive control model utilising these operator tools to simulate process control, obtained only a 5% improvement, achieving an 8-hours-ahead predictive accuracy of 35% ($\pm 7\%$) on future $P_{\text{slag}}$ values. The reason for this small improvement is the existence of a fundamental upper limit to predictive control improvement; control accuracy oscillates within a range best described as a damage-control range, with the input variables needed to facilitate process adjustments on a short term basis ($\leq 8$ hours) already in the furnace and no changes can be made to them.

- Fundamental design-, sampling- and process restrictions associated with the submerged arc furnaces limit the predictive and especially control accuracy or meaningfulness of any dynamic model - be it linear or non-linear.
11.2 Recommendations

The CFD model  The presented CFD model provides a well structured platform for solving steady-state furnace situations. It is a concrete first step in a CFD-type approach to understand and simulate the behaviour of phosphorus producing submerged arc furnace.

- The CFD model proves the existence of a narrow, gas-solid reduction zone where the bulk of the phosphorus is produced. This is an important insight.

- The upper boundary of this reduction zone is mainly determined by the chemical composition of the pellet, bed conductivity and bed permeability.

- The lower boundary of this reduction zone (and therefore the thickness thereof) is mainly determined by the structural qualities of the sintered pellet and the porosity of the pellet. At this point the reaction stops as shown in previous kinetic reduction studies done in projects (Dresen et al., 2002) (Van der Pas, 1999).

- Above this reduction zone, evidence was found of a thermal reserve zone similar to the one found in an iron blast furnace.

- Fast reaction rates in a narrow reaction band in combination with long residence times diminishes the influence changing reaction rates have on the process.

- Gaseous product and velocity information shows low, recirculating gaseous flow velocity areas that cause dust accumulation, thus resulting in increased pressure measurement in the outlet duct.

- Most of the heat exchanged between new pellets entering the furnace and the gaseous product gas produced in the reduction zone takes place in the top 0.5m of the furnace bed.

The importance of good quality data  Process data closer to actual values (and significantly different from the values used to construct the model) were introduced at a very late stage. The CFD model provided values closer to reality in three of the four major output variables. This concludes that the CFD model is robust, non-stiff (in a differential equation sense) and reflects reality.

11.2 Recommendations

All fundamental control decisions are taken as a result of slag analysis results. Therefore, it is vital that the analysis reflect the state of the slag as accurately as possible. The following simple, realistic recommendations could further improve understanding of the furnace and sharpen up control of the process.
Sampling

- Every slag sample submitted for analysis must contain four samples taken at equally spaced intervals (2 hours apart). If this is physically not possible (e.g. change of ladle, blocked slag hole etc.), it should be logged. The reason for not logging data is important and should be saved for future data mining. Hence this type of information should be made available on the data base.

- The current method of slag sampling is not good. The sampling process allows significant possibilities for contamination of the samples through impurities or through a frozen, previous sample. Especially in the iron industry, easy-to-use immersion slag samplers are being used on a regular basis to accurately take a slag sample fit for analysis.

- The last of the four slag samples, represents the most recent process history, while the first sample was taken 6 hours in the past. Owing to way the combined slag sample is prepared, differences in the mass of the individual four samples will affect the results in a proportional way. It is proposed that the four slag samples should be represented in the combined sample in a way that the last sample has more influence.

- The timestamp associated with the combined slag sample should not be the time of analysis but should carry the time when the sample was taken to ensure that dynamic models can be created.

- A more far reaching (and straight forward) recommendation is the analysis of slag samples every 4 hours, accompanied, of course, by the corresponding changes in feed mixture at the weighing stations. Such a measure would narrow the range of furnace control but will bring about extra costs.

User-developed software

- Use the in-Excel developed, data reconciliation software. This will utilise in-build soft-sensing capabilities. Amongst other benefits, it provides a third way of measuring the SPC of the furnaces in a online way. Developments and improvements to the Thermphos International database in recent years means that it is easy for continuously updated data to be e.g intelligently imported to a computer, the in-build data reconciliation macros activated and the soft-sensor values generated. With three SPC values available, a e.g. Kalman filter can calculate the most probable value (Maybeck, 1979).

- Utilise the in-Excel developed linear, dynamic model on a stand-alone computer and actively test predictive power. There are possibilities for the continuously-updated database to be accessed straight from level 2/3. Given the current 30% predictive accuracy, this exercise might seem redundant, but as measures are taken to re-define fundamental design, sampling and process limitation, the model may yet prove its worth.
11.2 Recommendations

The CFD model

- The modelling process is on-going and will require continuous aftercare; not only to generate results from the current model but also ensure its adaptability to changing process conditions.

- As additional information like mineralogy analysis of dig-out samples for temperature validation and reaction constants for new apatite feed material become available these new mathematical models can be implemented in order to improve the model.

- Perform accurate side cooling and electrode cooling temperature measurements to further optimise CFD model boundary fluxes.

- Factsage 5.4.1 (2006) is continuously updating its available databases. In the light of this, the should be further investigation of the heat capacity vs. time trends for the Moeller feed.

- The model does not yet include the full effect of coke (which has an effect on conductivity and permeability). The coke also provides the surface area for the P$_2$O$_5$ reaction to P$_4$. A next step would be to experimentally investigate the effect of varying coke particles on the conductivity and permeability of the Moeller bed.

Slightly more far reaching recommendations

- Silica does not have a substantial influence on the reaction within the bed, but it contributes to a large extent to the porous heterogeneity of the packed bed; pellets and cokes are all subject to screening, whereas the silica is not screened at all. It is proposed that a test be performed where the silica is pre-screened and only particles within a certain particle diameter range fed to the furnaces (first to the silo’s above the weighing stations. By improving the homogeneity of the bed the bed resistance can be stabilised and incidents of bridge formation and burden collapse can be minimised. Integrating silica in pellet as suggested by work of Prof M.A.Reuter and his students should be adopted, as this has had significant improvement of P recovery.

- Feed the coke directly to the reduction zone through hollow electrodes.

- Section 3.3 shows that the mechanical hoist restrictions imposed on the electrode operating heights may be one of the causes why the process deviates. How much the process will benefit from increasing the lower and upper set points for the movement of the electrodes?

- Section 3.3 also indicates that once a formed bridge collapses, cold Moeller will surround the electrode, causing the resistance around the electrode to increase and cause the sudden change in the electrode current. How much the process will benefit from electrodes that can vibrate? This might induce a series of controllable mini collapses underneath the electrodes and perhaps a more stable process.
Nomenclature

Arabic symbols

A  surface area [m^2]
a  absorption coefficient [-]
cos φ  power factor [-]
Cp_{pb}  heat capacity of the packed bed (Moeller) [\text{J/kg/K}]
DDS  dynamic-driven state
FDF  the ratio used in the CFD model calculation in order to account for the gas formation and subsequent decrease in packed bed mass flowrate [-]
FOG  the additional gas from the furnace after the phosphorus has been extracted
fr  the fraction of available furnace volume occupied by freezeling [%]
H_R  enthalpy changes as a result of the energy required for the main chemical reaction [\text{J/kg P_2O_5}]
I  current [Ampere]
J_{ij}  the objective function for the i’th elements in the j’th stream [-]
J_{tot}  the total objective [-]
k_{eff}  effective thermal conductivity coefficient (user-defined model) [\text{W/m.K}]
k_{cond}  thermal conductivity coefficient [\text{1/kg.K}]
L  length [m]
m_{Ferro}  ferrophosphorus flowrate [\text{kg/s}]
m_{Slag}  slag flowrate [\text{kg/s}]
m_{UnrCoke}  flowrate of the unreacted coke [\text{kg/s}]
m_{P_4}  flowrate of P_4 [\text{kg/s}]
m_{Moeller}  flowrate of the Moeller feed material through the furnace [\text{ton/hour}]
$P_2O_5^{m}$ a downward mass flowrate that transports the concentration scalar ($P_2O_5$) down throughout the packed bed domain [kg/s]

$P_2O_5^S$ a scalar value representing $P_2O_5$ concentration in the packed bed

$P_2O_5^{(pellets)}$ the amount of $P_2O_5$ present in the pellets in the Moeller [wt%]

$P_2O_5^{(slag)}$ the amount of $P_2O_5$ present in the slag [wt%]

$P$ electrical power [Watt]

$q$ heat flow [Watt]

$Q_{feedchutes}$ The energy required to heat up the Moeller from 40° approximately 300° when it enters the furnace [MegaWatt]

$Q_R$ energy required for the main chemical reaction [W]

$Q_{Total}$ the total amount of energy supplied to the furnace through the electrodes [MegaWatt]

$Q_{HM}$ energy required for heating and melting of the packed bed [$\frac{Watt}{m^3}$]

$s$ scattering coefficient [-]

SPC specific power consumption $[\frac{MW\cdot h}{ton \ P_4}]$

$T_{cell}$ the temperature of each individual cell in the model grid [K]

TDS thermodynamic-driven state

$T_{gas}$ outlet temperature of the gaseous product as it leaves the outlet pipes [K or °C]

$Tot_{elec}$ energy input to the model [Watt]

UDS user-defined scalar defined within Fluent 6.1.18 (2003)

$V_{arc}^{1,2,3}$ the volumes of the arc zones created underneath the electrodes for the introduction of power to the furnace [m$^3$]

$V_{cell}$ the volume of the individual control volumes within the packed bed domain as created by grid generation program [m$^3$]

$V$ voltage [Volt]

$V_{pb}$ volume of the packed bed in the furnace [m$^3$]

$W$ a velocity vector in the downward direction equal to the packed bed speed of descend [$\frac{m}{s}$]

$z_{cell}$ the height of each individual cell in the model grid [m]
11.2 Recommendations

$z_i$  $z$ coordinate of sphere $i$ centroid [m]

**Greek symbols**

$\Delta T_{\text{cell}z}$ temperature gradient within each cell in the downward (z) direction [°C]

$\Delta T_{\text{dust}}$ temperature difference between the inlet and outlet slag tap hole cooling water [°C]

$\phi_{\text{pb}}$ void fraction of the packed bed (porosity) [-]

$\rho$ density [kg m$^{-3}$]

$\rho_{\text{pb}}$ bulk density of the packed bed [kg m$^{-3}$]

$\phi$ phase angle between the voltage and current [-]

$\tau_{\text{afterRZ}}$ residence time of the material from the reduction zone until it exits the furnace [hours]

$\tau_{\text{beforeRZ}}$ residence time of the material from the top of the packed Moeller bed in the furnace until it reaches the reduction zone [hours]

$\tau_{\text{feedchutes}}$ residence time of the material from the weighing station, through the feed pipes until it enters the furnace [hours]

$\tau_{\text{furnace}}$ residence time of the feed material inside the furnace [hours]

$\tau_{\text{tot}}$ residence time of the material from the weighing station, through the feed pipes until it exists the furnace [hours]

$\rho_{\text{bulk}}$ the bulk density of the packed bed [kg m$^{-3}$]

$\sigma$ standard deviations
Bibliography


Appendix A

Basic data reconciliation theory

Methods of data reconciliation The two methods for data reconciliation that appear to find favour among the researchers in minerals processing are either the Lagrange Multiplier technique or a direct minimisation technique of the variance weighted sum of square error which work on the independent variables. The direct minimisation techniques may employ a number of non-linear programming (NLP) algorithms such as any of quadratic programming (QP), sequential quadratic programming (SQP), the generalised reduced gradient method (GRG) which implicitly uses Newtons method, or random search methods, each algorithm having each own set of advantages and disadvantages. An evaluation of the algorithms, based on efficiency, reliability, global convergence, performance in solving degenerate problems, performance in solving ill-conditioned problems, performance in solving indefinite problems, sensitivity to variations in the problem and ease of use, has shown that the GRG and SQP methods significantly outperformed the other algorithms (Ekesteen, Frank and Reuter, 2004). In this report, a direct minimisation technique of the variance weighted sum of square error was used to reconcile the data. The GRG non-linear optimization code is described by Edgar and Himmelblau (2001) and is incorporated into Microsoft Excel Solver Platform, the tool used in the optimisation procedure in this thesis. A full theoretical discussion on the GRG algorithm can be found in Edgar and Himmelblau (2001) and will not be repeated here.

Constructing the objective function Improved data through reconciliation are defined as the optimal solution to a constrained least squares or maximum likelihood objective function. The measured values of streams (flowrates, elemental composition) of a process never satisfy constraints of material conservation because of the uncertainties in the measurements, expressed in the standard deviations of the measured flowrates and compositions. These measured values are represented by $\bar{Q}_{ij}$, where $i =$ counter or index representing the flowrate of individual elements and $j =$ counter of index representing the flowrate of a particular stream. The estimated values (estimators) of these streams (flowrates, elemental compositions) can be calculated taking into account the accuracy, or standard deviation, attached to each measurement. These estimated values are represented by $Q_{ij}$. The standard deviations are the known uncertainties that exist for the streams and are represented by $\sigma_{ij}$. These standard deviations are discussed in Section 5.3.3. The objective function
for a specific element in a specific stream can now be constructed and is given in Equation A.1.

\[ J_{ij} = \left( \frac{Q_{ij} - \bar{Q}_{ij}}{\sigma Q_{ij}} \right)^2 \]  

(A.1)

From Equation A.1 the total objective function for m amount of streams and n amount of elements are depicted in Equation A.2

\[ J_{\text{tot}} = \sum_{j=1}^{m} \sum_{i=1}^{n} (J_{ij}) \]  

(A.2)

Mathematically, the GRG algorithm is then utilised in order to minimise the total objective function through adjustments to the estimated values (Q_{ij}). These adjustments do not have total freedom and are guided within certain restrictions or constraints.
Appendix B

Data reconciliation and accompanying software development

The reconciliation of Thermphos International data was performed using Excel. The following figures provide a brief visual overview of the procedure.
## Data reconciliation and accompanying software development

**Figure B.1:** The filtered flowrate data are placed in this sheet with every timestamp attached. By pressing the button depicted at the top of the picture, the reconciliation process commences. The reconciliation macro starts by copying the first row of data to the sheet depicted in Figure B.2.
The reconciliation macro is started from within the sheet seen in Figure B.1 and the copied flowrates are used as initial values for the mass balance. The next step in the reconciliation process is to minimise the objective functions given standard deviation values for every variable. These are shown in Figure B.3.
Figure B.3: Every variable has a standard deviation value that reflects the accuracy of the measurement. Notice the 16% standard deviation of the $P_2O_5$ content in the slag and the exceptionally high standard deviation values for the unmeasured gaseous output variables.
Appendix C

Basic theory of the ARX-type model

The acronym ARX is shorthand notation for Auto Regressive with eXogenous input(s). When looking at transfer function models, of which ARX is a part of, the linear relationship between the current output, \( y(t) \), a definite number of past outputs, \( y(t-1) \) (the Auto Regressive part), and inputs, \( u(t-k) \) (the eXogenous part), the general ARX model structure can be written as the following differential equation:

\[
y(t) = -a_1 y(t-1) - \ldots - a_{na} y(t-na) + b_1 u(t-nk) + \ldots + b_{nb} u(t-nk-nb+1) + e(t) \tag{C.1}
\]

For Equation C.1 to be used in prediction, the \( e(t) \) must, however, be omitted! The reason for this is that the signal, \( e(t) \), which represents noise that cannot be predicted, since it is independent of everything that has happened before.

\[
y(t) = -a_1 y(t-1) - \ldots - a_{na} y(t-na) + b_1 u(t-nk) + \ldots + b_{nb} u(t-nk-nb+1) \tag{C.2}
\]

The structure is entirely defined by the three integers \( na \), \( nb \) and \( nk \). The terms \( na \) and \( nb \) are called the order of the input and output respectively. They define how many past input/output variables are taken along in the model. The term \( nk \) is the time-delay (or residence time in the context of this report) of the model. The time it takes for an input to have an effect on the output.

For models that have multiple input variables, \( nb \) and \( nk \) are row vectors instead of numbers. The coefficients of the vectors correspond to one of the time series of the input. The \( i_{th} \) element gives the order or delay associated with the \( i_{th} \) input. The predictive, ARX structure for a one-output, multiple-input and no time delay (\( nk = 0 \)) is as follows:
\[ y(t) = -a_1 y(t - 1) - \ldots - a_{na} y(t - na) + B_0 u(t) + B_1 u(t - 1) + \ldots + B_{nb} u(t - nb) \] (C.3)

After optimising the coefficients of B by linear regression, using the least squares estimations method, the output is described best by that combination of input for that specific model structure. In practice, this means that all input time series get a pinned weight, which defines their influence to the output. The model is therefore fit for handling data with a pinned relation of input and output, but is inflexible towards process changes. If therefore, like at Thermphos International, the characteristics of the process also changes with time, the parameters of the model are to be estimated recursively and is called an adaptive model (see Section 6.2).

By increasing the number of na and nb (and therefore the order of the model), more past input and output variables are considered. This could be beneficial to the accuracy, but could also increase the model complexity, computation time and result in overtraining, or overfitting. Overfitting is fitting a model that has too many parameters. An absurd and false model may fit perfectly if the model has enough complexity by comparison to the amount of data available.

**Overfitting**

Overfitting is generally recognized to be a violation of Occam’s razor (Gams, 2001). The concept of overfitting is important also in machine learning (see Section 6.9). Usually a learning algorithm is trained using some set of training examples, i.e. exemplary situations for which the desired output is known. The learner is assumed to reach a state where it will also be able to predict the correct output for other examples, thus generalizing to situations not presented during training. However, especially in cases where learning was performed too long or where training examples are rare, the learner may adjust to very specific random features of the training data, that have no causal relation to the target function. In this process of overfitting, the performance on the training examples still increases while the performance on unseen data becomes worse.

For an informed choice on the best model order, knowledge of the process and especially the history associated with the data become crucial. Section 7.2 investigates the subsequent choice of model order, as well as expanding on this development and validation processes.
Appendix D

Dynamic model and accompanying software development

After reconciliation, the data are ready for dynamic model development. The dynamic model was trained and validated in two different platforms; Matlab and Microsoft Excel. The main sheet associated with the Microsoft Excel model are shown here.
Averages
0.6 1.7 2.1 442.6 413.4 69.1 71.8 55.8 5.6 5.5 4.9 1.8 0.9 0.5 0.3 0.3 260.0 30.3
Standard deviation
0.2 0.9 1.8 138.0 154.9 18.9 13.4 15.5 6.0 3.4 3.5 0.2 0.0 0.0 0.0 0.0 77.4 1.5

Future data
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Present data
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
Past data
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

Time
C-Mn
C-Ti
C-Si
E-TempA
E-TempB
E-oh-L
E-oh-M
E-oh-R
E-mohm-L
E-mohm-M
E-mohm-R
F-MWh/Moeller
C-Bas
C-fix
C-P2O5-pellets
C-BasM
F-Moeller
C-Gravelfactor

Predicted P2O5 in slag
Actual P2O5 in slag
Error
(Error)^2
Sum of squared error & objective function to be minimised

Figure D.1: These 18 input variables used to train and validate the dynamic model is seen here. The sum of squared error or objective function to be minimised is shown. Figure 7.4 shows the standardised influence that these 18 input variables had on predicting the $P_{2O5}^{(slag)}$. 
Appendix E

CFD model and accompanying software development

For Thermphos International to access and interpret the various CFD modelling scenario’s in an effective way a special tool was developed in Microsoft Excel. This standard spreadsheet contains seven individual sheets. The rest of Appendix E explains the aim of these seven sheets accompanied by relevant figures showing the individual sheets (of Scenario 3). Some general information before proceeding to the individual explanations of the sheets:

- Only the cells with white writing and a black background should be changed by the user.
- Each scenario from Chapter 10 has it’s own Excel file

These following can be said about the seven sheets within the Excel file:

1. CFD model summary: In this sheet represented by Figures E.1 and E.2, all important results are summarised. All values are updated automatically and the user will not have to change the values in any of these cells directly. The functions and equations used have all been covered in this study.

2. CFD model scenarios: In this sheet represented by Figures E.3 and E.4 all the various scenarios described in Chapter 10 are listed. The reader can identify all the parameters associated with each scenario as well as the variables used for sensitivity analyses. Every new scenario created by future users can be added to the list.

3. Mass balance: This sheet represented by Figures E.6 and E.7 performs the necessary calculations in order to prepare the mass balance as described in Section 9.2. The user can obtain the necessary input values from a standard, 8-hourly Thermphos International analysis. Some assumptions are also required about the wt% of fluoroapatite, hydroapatite and wollastonite in the pellets (after sintering). The user can also use this sheet to prepare a theoretical mass balance based on a new feed material or different C-fix value. For this purpose the user can call on a series of macro contained in the sheet.
4. **Factsage input**: This sheet represented by Figure E.8 utilises data from the *Mass balance* sheet to prepare the data for the *Factsage 5.4.1* (2006) module. This is done through a macro activated by the blue button seen in the figure. Both Figure 9.11 and Figure 9.12 are generated from data prepared in this sheet.

5. **Fluent and C++ input values**: This sheet represented by Figures E.9, E.10 and E.11 give the input variables used in *Fluent 6.1.18* (2003) and in the additional C++ code seen in Appendix F. Important parameters include the individual arc zone volumes shown in Figure 9.3, the densities of the feed material, the individual power inputs of the electrodes (see Section 9.5.1), the scalar value \(P_{2O_5}\) discussed in Section 9.7.1 and the boundary condition values as discussed in Section 9.5.4, 9.5.5, 9.5.6 and 9.5.7.

6. **CFD model results input**: This sheet represented by Figure E.12 is the sheet were all the output results from *Fluent 6.1.18* (2003) are filled in. The sheet include screen-capture pictures of exactly where in *Fluent 6.1.18* (2003) the user must obtain the output data.

7. **CFD model pictures**: This sheet represented by Figure E.14 gives the opportunity to display some resulting pictures from the model. These pictures must be selected, copied and pasted by the user.
Figure E.1: A complete summary of the CFD modelling results from Scenario 3. Clearly circled are the gaseous outlet temperature, the slag temperature, the SPC(in), the SPC(out) and the $P_2O_5_{(slag)}$ value.
Figure E.2: An additional summary of the CFD modelling results from Scenario 3, showing each zone within the furnace.
Figure E.3: The different scenarios used throughout this study. An explanation of the different codes associated with the various scenarios can be seen in Figure E.4.
Figure E.4: An explanation of the different codes associated with the various scenarios seen in Figure E.3.
Figure E.5: The various electrode operating heights used in this study
**Figure E.6:** The chemical analysis and mass balance values of the feed.
Figure E.7: The chemical analysis and mass balance values of the feed.
Table E.9: This sheet is used to prepare the data for the Factsage 5.4.1 (2006) module.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Initial</th>
<th>Final</th>
<th>Reaction</th>
<th>Initial</th>
<th>Final</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO2Fe2</td>
<td>99.0</td>
<td>100.0</td>
<td>Fe2O3</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>FeO</td>
<td>0.0</td>
<td>0.0</td>
<td>Fe2O3</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Fe2O3</td>
<td>0.0</td>
<td>0.0</td>
<td>Fe2O3</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>FeO</td>
<td>0.0</td>
<td>0.0</td>
<td>Fe2O3</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

The feed for Factsage given = 1kg P2O5
**FLUENT & C++ INPUT VALUES**

**Moeller feed before entering the feed pipes**

| Temperature | 313 K |

**Packed bed**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>37.7%</td>
</tr>
<tr>
<td>Density</td>
<td>1043 kg/m³</td>
</tr>
<tr>
<td>Bulk density</td>
<td>1148 kg/m³</td>
</tr>
<tr>
<td>Packed bed volume</td>
<td>196.6 m³</td>
</tr>
<tr>
<td>Packed bed AND Slag volume</td>
<td>228.0 m²</td>
</tr>
<tr>
<td>Packed bed surface</td>
<td>59.6 m²</td>
</tr>
<tr>
<td>Vertical distance from top Muller to bottom Slag</td>
<td>3.83 m</td>
</tr>
</tbody>
</table>

**Inlet volume of LEFT inlet zone**

<table>
<thead>
<tr>
<th>Volume</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet volume of LEFT inlet zone</td>
<td>1.47</td>
</tr>
<tr>
<td>Inlet volume of MIDDLE inlet zone</td>
<td>1.67</td>
</tr>
<tr>
<td>Inlet volume of RIGHT inlet zone</td>
<td>1.31</td>
</tr>
</tbody>
</table>

**Moeller feed as it enters the furnace**

| Temperature | 573 K |

**Pellets**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>wt% in feed</td>
<td>18.94%</td>
</tr>
<tr>
<td>Density</td>
<td>1714 kg/m³</td>
</tr>
<tr>
<td>Porosity</td>
<td>44%</td>
</tr>
</tbody>
</table>

**Grind**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>wt% in feed</td>
<td>20.27%</td>
</tr>
<tr>
<td>Density</td>
<td>2600 kg/m³</td>
</tr>
</tbody>
</table>

**Coke**

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>wt% in feed</td>
<td>10.70%</td>
</tr>
<tr>
<td>Density</td>
<td>12.80 kg/m³</td>
</tr>
<tr>
<td>Porosity</td>
<td>34%</td>
</tr>
</tbody>
</table>

**Slag**

| Weight % of coke that leave with the slag | 0.00% |

These three values (B:16-18) are filled in by the user, obtained from Fluent and depends on which electrodes structure is used (E1,E2 etc.)

The density values in cells B:23, B:28 and B:32 can be changed by the user.

**Figure E.9:** Input variables used in Fluent 6.1.18 (2003) and in the additional C++ code. This is the first part of the sheet named Fluent and C++ input values. Important parameters include the individual arc zone volumes shown in Figure 9.3 and the densities of the feed material.
User Defined Scalar

- wt% P2O5 in pellets: 20.08%
- Scalar value in Fluent to be retained: 0.01 kg of P2O5/m³
- Flowrate of Moeller feed: 10.52 kg/h

Packed bed velocity (before onset of reduction)

- Downwash velocity: 1.938 m/s
- Residence time of pellet within reactor: 8.91 hours

Energy required to heat the Moeller to furnace inlet temp.

- Energy added to electrode cooling to compensate for the heating of the Moeller to the furnace inlet temperature: 2.955 MW

Energy & mass inputs for inlet zones

<table>
<thead>
<tr>
<th>Additional gas inlet for the model</th>
<th>1.18 kg/m³/s</th>
<th>kg/kg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy supplied to LEFT inlet zone</td>
<td>9.624 MW/m³</td>
<td>0.195</td>
</tr>
<tr>
<td>Energy supplied to MIDDLE inlet zone</td>
<td>11.510 MW/m³</td>
<td>0.146</td>
</tr>
</tbody>
</table>

Packed bed velocity (after reduction)

- Flowrate of the drag and the coke: 7.26 kg/m³/s
- Downwash velocity: 1.938 m/s

Wohler reaction inside the packed bed

- Onset temperature of Wohler reaction: 483.8 K

This value is filled in by the user and the different values can be obtained from the "mass balance" tab (cells D:4-9). Other values are also possible.

**Figure E.10:** Input variables used in *Fluent 6.1.18* (2003) and in the additional C++ code. This is the second part of the sheet named *Fluent* and C++ input values. Important parameters include the individual power inputs of the electrodes (see Section 9.5.1) and the scalar value (P2O5) discussed in Section 9.7.1.

**Figure E.11:** Input variables used in *Fluent 6.1.18* (2003) and in the additional C++ code. This is the third part of the sheet named *Fluent* and C++ input values. Important parameters include the boundary condition values as discussed in Section 9.5.4, 9.5.5, 9.5.6 and 9.5.7.
Figure E.12: The top part of this sheet is used by the user to enter the Fluent 6.1.18 (2003) results. The values are copied automatically to the correct sheets. The rest of this sheet provides screen-captured examples of how to obtain the correct data.
Figure E.13: This picture provides the last piece of the sheet shown in Figure E.12.
Figure E.14: Selected pictures from Fluent 6.1.18 (2003).
CFD model and accompanying software development
Appendix F

CFD source code

All user-defined functions described in this study were programmed in C++ code and provided below.
Velocity vector, with only downward direction defined.

Scalar density defined as = 1

FDF

Figure F.1: Page 1 of 7 of the C++ source code
DEFINE_SOURCE(mass_inlet_right,c,t,dS,eqn)
{
    real source13;
    source13 = GAS_INLET_RIGHT;
    C_UDMI(c,t,26) = source13;
    return source13;
}

DEFINE_SOURCE(energy_pb,c,t,dS,eqn)
{
    real reaction, reaction_slag, y;
    real source4, packedbed, cp_packedbed;
    real packedbed_NORMAL, packedbed_ABNORMAL;
    real packedbed_NORMAL_less, packedbed_ABNORMAL_less;
    real packedbed_NEW_FEED, cp_pb_int, cp_pb_int_573K;
    real cp_pb_int_313K;
    real cp_pb_int_313K_853K;
    real cp_pb_int_854K;
    real cp_pb_int_313K_1323K;
    real cp_pb_int_1324K;
    real cp_pb_int_313K_1373K;
    real cp_pb_int_1374K;
    real cp_pb_int_313K_1463K;
    real cp_pb_int_1464K;
    real cp_pb_int_313K_1523K;
    real cp_pb_int_1524K;
    real cp_pb_int_313K_1753K;
    real cp_pb_int_1754K;
    real cp_pb_int_313K_2003K;
    real cp_pb_int_2004K;
    real cp_pb_int_313K_3500K;
    real MaseHare1;
    real MaseHare2;
    real MaseHare3;
    real MaseHare4;
    real MaseHare5;
    real MaseHare6;
    real MaseHare7;
    real MaseHare8;
    real MaseHare9;
    real MaseHare10;
    real MaseHare11;
    real MaseHare12;
    real MaseHare13;
    real MaseHare14;
    real MaseHare15;
    real MaseHare16;

Figure F.2: Page 2 of 7 of the C++ source code
real temp = C_T(c,t);
real x[ND_ND];

C_CENTROID(x, c, t);
y = x[2];
if (temp < 313.)
{cp_packedbed = 889.0;
cp_pb_int = 0.;}
if (temp >= 313. & & temp < 854.)
{cp_packedbed = MaseHare2 + MaseHare1*temp;
cp_pb_int = ((MaseHare1/2)*pow(temp,2) + (MaseHare2*temp)) - cp_pb_int_313K;}
if (temp >= 854. & & temp < 1324.)
{cp_packedbed = MaseHare4 + MaseHare3*temp;
cp_pb_int = (((MaseHare3/2)*pow(temp,2))+(MaseHare4*temp))-cp_pb_int_854K+cp_pb_int_313K_853K;}
if (temp >= 1324. & & temp < 1374.)
{cp_packedbed = MaseHare5*temp + MaseHare6;
cp_pb_int = (((MaseHare6/2)*pow(temp,2))+(MaseHare6*temp))-cp_pb_int_1324K+cp_pb_int_313K_1323K;}
if (temp >= 1374. & & temp < 1464.)
{cp_packedbed = MaseHare7*temp + MaseHare8;
cp_pb_int = (((MaseHare7/2)*pow(temp,2))+(MaseHare8*temp)) - cp_pb_int_1374K + cp_pb_int_313K_1373K;}
if (temp >= 1464. & & temp < 1524.)
{cp_packedbed = MaseHare9*temp - MaseHare10;
cp_pb_int = (((MaseHare9/2)*pow(temp,2))-(MaseHare10*temp))-cp_pb_int_1464K+cp_pb_int_313K_1463K;}
if (temp >= 1524. & & temp <= 1573.)
{cp_packedbed = MaseHare11*temp + MaseHare12;
cp_pb_int = (((MaseHare11/2)*pow(temp,2))+(MaseHare13*temp))-cp_pb_int_1524K+cp_pb_int_313K_1523K;}
if (temp >= 1574. & & temp < 2004.)
{cp_packedbed = MaseHare13*temp + MaseHare14;
cp_pb_int = (((MaseHare13/2)*pow(temp,2))+(MaseHare14*temp)) - cp_pb_int_1574K + cp_pb_int_313K_1573K;}
if (temp >= 2004.)
{cp_packedbed = MaseHare15*temp + MaseHare16;
cp_pb_int = (((MaseHare15/2)*pow(temp,2))+(MaseHare16*temp)) - cp_pb_int_2004K + cp_pb_int_313K_2003K;}

if (y < -1.5 & & y > -1.75)
{
cp_pb_int_573K = 219310.;
if (temp > 573.0)
{packedbed_NEW_FEED = (cp_pb_int - cp_pb_int_573K) * RHO_PACKEDBED * (1/0.075) * W;
C_UDMI(c,t,10) = packedbed_NEW_FEED;
packedbed = packedbed_NEW_FEED;} if (temp <= 573.0)
{ packedbed = 0.0;}}
if (y <= -1.75)
{
if (C_T_RG(c,t)[2] <= 0)
{
if (C_T(c,t) <= 1423.0)
{packedbed_NORMAL = -cp_packedbed) * RHO_PACKEDBED * C_T_RG(c,t)[2] * W;
C_UDMI(c,t,22) = packedbed_NORMAL;
packedbed = packedbed_NORMAL;}
if (C_T(c,t) > 1423.0)
{packedbed_NORMAL_less = -(cp_packedbed) * RHO_PACKEDBED * C_T_RG(c,t)[2] * W * FLOWRATE_DECREASE_FACTOR;
C_UDMI(c,t,22) = packedbed_NORMAL_less;
packedbed = packedbed_NORMAL_less;}}

Figure F.3: Page 3 of 7 of the C++ source code
if (C_T_RG(c,t)[2] > 0)
{
    if (C_T(c,t) <= 1423.0)
    {
        packedbed_ABNORMAL = -(cp_packedbed) * RHO_PACKEDBED * C_T_RG(c,t)[2] * W;
        C_UDMI(c,t,12) = packedbed_ABNORMAL;
        packedbed = packedbed_ABNORMAL;
    }
    if (C_T(c,t) > 1423.0)
    {
        packedbed_ABNORMAL_less = -(cp_packedbed) * RHO_PACKEDBED * C_T_RG(c,t)[2] * W * FLOWRATE_DECREASE_FACTOR;
        C_UDMI(c,t,23) = packedbed_ABNORMAL_less;
        packedbed = packedbed_ABNORMAL_less;
    }
}

if ((C_T(c,t) <= 1173.))
{
    reaction_slag = 0.0;
}
if ((C_T(c,t) > 1173.) && (C_T(c,t) <= 1285.))
{
    reaction_slag = -((3.97e6 + 4.61e6 + 4.9e6 + 5.22e6 + 5.54e6 + 5.89e6 + 8.32e6)/7) * C_VOLUME(c,t);
    C_UDMI(c,t,18) = reaction_slag;
    if ((C_T(c,t) <= 1422.))
    {
        reaction_slag = 0.0;
    }
    if ((C_T(c,t) > 1422.) && (C_T(c,t) <= 1473.))
    {
        reaction = -7.233e6 * C_UDMI(c,t,0);
        if ((C_T(c,t) > 1473.) && (C_T(c,t) <= 1523.))
        {
            reaction = -10.912e6 * C_UDMI(c,t,0);
            if ((C_T(c,t) > 1523.) && (C_T(c,t) <= 1573.))
            {
                reaction = -13.040e6 * C_UDMI(c,t,0);
                if ((C_T(c,t) > 1573.) && (C_T(c,t) <= 1623.))
                {
                    reaction = -13.554e6 * C_UDMI(c,t,0);
                    if ((C_T(c,t) > 1623.) && (C_T(c,t) <= 1723.))
                    {
                        reaction = -14.327e6 * C_UDMI(c,t,0);
                        if ((C_T(c,t) > 1723.))
                        {
                            reaction = -16.31e6 * C_UDMI(c,t,0);
                        }
                    }
                }
            }
        }
    }

Figure F.4: Page 4 of 7 of the C++ source code
source4 = reaction + packedbed + reaction_slag;
C_UDMI(c,t,3) = cp_packedbed;
C_UDMI(c,t,4) = packedbed;
C_UDMI(c,t,5) = C_T_RG(c,t)[2];
C_UDMI(c,t,6) = reaction;
C_UDMI(c,t,9) = source4;
return source4;
}

DEFINE_SOURCE(enrg_inletALL,c,t,dS,eqn)
{
    real furnace_inputALL, source10;
    real temp = C_T(c,t);
    furnace_inputALL = (11.510e6);
    source10 = furnace_inputALL;
    C_UDMI(c,t,15) = furnace_inputALL;
    return source10;
}

DEFINE_SOURCE(enrg_inlet_left,c,t,dS,eqn)
{
    real furnace_input1, source6;
    real temp = C_T(c,t);
    furnace_input1 = (10.221e6);
    source6 = furnace_input1;
    C_UDMI(c,t,7) = furnace_input1;
    return source6;
}

DEFINE_SOURCE(enrg_inlet_middle,c,t,dS,eqn)
{
    real furnace_input2, source8;
    real temp = C_T(c,t);
    furnace_input2 = (9.663e6);
    source8 = furnace_input2;
    C_UDMI(c,t,13) = furnace_input2;
    return source8;
}

DEFINE_SOURCE(enrg_inlet_right,c,t,dS,eqn)
{
    real furnace_input3, source9;
    real temp = C_T(c,t);
    furnace_input3 = (11.510e6);
    source9 = furnace_input3;
    C_UDMI(c,t,14) = furnace_input3;
    return source9;
}

Figure F.5: Page 5 of 7 of the C++ source code
DEFINE_UDS_FLUX(burden_flux,f,t,i)
{
  float NV_VEC(psi), NV_VEC(A);
  NV_D(psi, U, V, W);
  NV_S(psi, "d, RHO");
  F_AREA(A, f, t);
  return NV_DOT(psi, A);
}

DEFINE_PROPERTY(eff_therm_cond, c, t)
{
  real etc, y, y_horizontal, x_horizontal;
  real x[ND_ND];
  C_CENTROID(x, c, t);
  y = x[2];
  y_horizontal = x[1];
  x_horizontal = x[0];

  if (y <= -1.5)
  {
    if (temp > 2700.)
      etc = 3000;
    if (temp <= 2700. && temp > 1000.)
      etc = (9.47e-10*pow(temp,3) - 1.15e-6*pow(temp,2) + 5.13e-3*temp - 1.70);
    if (temp <= 1000.)
      etc = (1.09e-6*pow(temp,2) + 1.57e-3*temp + 4.21e-1)*1.5*2.5;
  }

  if (y > -1.5)
  {
    etc = 0.06;
  }

  C_UDMI(c, t, 8) = y;
  C_UDMI(c, t, 16) = y_horizontal;
  C_UDMI(c, t, 17) = x_horizontal;
  return etc;
}

DEFINE_PROPERTY(absorp_coeff, c, t)
{
  real etc, y, y_horizontal, x_horizontal, abs_coeff;
  real temp = C_T(c, t);
  real x[ND_ND];
  C_CENTROID(x, c, t);
  y = x[2];
  y_horizontal = x[1];
  x_horizontal = x[0];

  if (y <= -1.5)
  {
    abs_coeff = 1.6;
  }

  if (y > -1.5)
  {
    abs_coeff = 0.128;
  }

  C_UDMI(c, t, 19) = abs_coeff;
  return abs_coeff;
}

Figure F.6: Page 6 of 7 of the C++ source code
DEFINE_PROPERTY(scatt_coeff, c, t)
{
    real etc, y, y_horizontal, x_horizontal, scatt_coeff;
    real temp = C_T(c, t);
    real x[ND_ND];
    C_CENTROID(x, c, t);
    y = x[2];
    y_horizontal = x[1];
    x_horizontal = x[0];

    if (y <= -1.5)
    {
        scatt_coeff = 0.95;
    }
    if (y > -1.5)
    {
        scatt_coeff = 0.2;
    }
    C_UDMI(c, t, 21) = scatt_coeff;
    return scatt_coeff;
}

DEFINE_PROFILE(porosity_bed, t, i)
{
    real x[ND_ND], y;
    cell_t c;

    begin_c_loop(c, t)
    {
        C_CENTROID(x, c, t);
        y = x[2];
        F_PROFILE(c, t, i) = 0.0178*y + 0.4037;
        end_c_loop(c, t))

Figure F.7: Page 7 of 7 of the C++ source code
Appendix G

Acknowledgements

I will never forget my first morning in The Netherlands. A strange, low frequency noise started seeping into my dream as I slept on the 4th floor of a hotel long since swallowed up by DuWo. I opened my eyes, lifted the covers, stumbled across the busy carpet, pulled back the curtain, opened the door and stepped onto the crisp balcony - just in time to see a long and heavily loaded boat slowly crawling through town!

Like that boat, my PhD journey sometimes felt pretty long and heavily loaded - crawling along at a steady, but tediously slow pace. The route to my (all) final (PhD) destination(s) was uncharted and trial-and-error characterised my voyage. Some days were also spent waiting for bridges to open, water levels to rise and various reconstruction projects to be completed. Yet, I always knew that a short and light boat could speed up the journey, but ultimately deliver nothing!

Finally, on 26 June 2008, I arrive at my destination. I go ashore and sit down on a wooden bench in the bright sunshine. The ducks quickly approach as I take out my sandwiches. The boat is fixed to the jetty and all my cargo will be unloaded in precisely one hour. As I gaze back at the boat I spent so much time on, I see my various clients inspecting their consignment, nodding their heads approvingly. Not surprising, though, considering that my clients travelled with me every inch of the way! In fact, my boat was absolutely loaded with people from bow to stern. Some accompanied me for only parts of the way, while others accompanied me for the entire journey. Without these people, there would have been no voyage. I watch them as they leave the boat...

I met Eleonora Simeone on the 13th of November 2003 and she met me on the 18th of November 2003... In her defense, that was the day she arrived at Resource Engineering (part of Technical Earth Sciences) and she was introduced to many people on that day. We quickly shared stories, later an apartment and finally our lives - together with our Cinzia.

"Ele, I found in you a wonderful partner.
Thank you so much for all you support, love and understanding during my (our) journey.
If I can support you in your PhD journey half as well as you supported me, you will have an easy ride in."
My parents, Emil and Hetsie Scheepers, met me on the 5th of March 1975 and, if memory serves, I met them roughly three years later. They were tall, always hanging around and trying to teach me stuff all the time. Some of it never stuck, like the lesson never to drink milk straight from the carton. Luckily for me, some of it did stick. Attributes like perseverance, patience and respect made it all the way to 2008.

"Pa en Ma, baie dankie vir ontelbare opofferings. Sonder julle was ek nogsteeds op die 4de vloer."

I met my sister Marisa, and my brothers Rudi and Marco, as they came out. We have since shared our lives through thick and thin. Marisa was later joined by Bertrand and even later by little Tijs, my beautiful nephew. Marco was joined by Mary-Ann, while Rudi is joined by someone else every week.

"Sommer net dankie! Dit is absoluut heerlik om saam met julle groot te word."

Markus Reuter and I met each other on the same day in 2002. He was (and is) a brilliant academic and dynamic person that impressed me straight away. When he accepted my PhD application a couple of months later, I was ecstatic. He had looked beyond my late nights and lukewarm grades! Thus began our long road together. When Markus and his family moved to Australia, he always stayed true to his promise; remaining on my boat and guiding me through to the end of my journey.

"Markus, jy bly die beste ingenieur wat ek nog ooit ontmoet het. Baie baie dankie vir jou ondersteuning deur hierdie jare. Sonder jou was ek nooit eers op die 4de vloer nie."

Yongxiang Yang and I met in South Africa. It was a pleasant sunny day and we shared a cup of tea. During the next couple of years and with a thoughtful blend of warmth, patience and insight, Yongxiang helped me through good times as well as testing times.

"Thank you for all our talks and productive CFD discussions, Yongxiang. We finally made it."

Halfway through my PhD I (we) found a home with Rob Boom at LMP. During the next couple of years, Rob allowed me to follow my research instincts, while at the same time keeping a watchful eye.

"Hartelijk bedankt Rob. Ik zal je altijd onthouden als stabilité gedurende een turbulente tijd."

Greg Georgalli was always kinda there - there in the way that a radio station is all around you, providing that you tune in. Well, I tuned in! However, six months before my departure to The Netherlands transmission stopped. He was too busy being a pioneer, blazing his own trail in The Netherlands and - in the process - making it all so much easier for me. Together with Alet Nienaber we learnt, we laughed and we had a couple of drinks.
I met my second family, Nicola Simeone, Nina Logoluso, Giuditta Simeone and Miki Simeone, on my first wide-eyed visit to Rome. They took one look at me and - despite what they saw - decided to open their homes as well as their hearts to me. Petrit and Giuditta are also starting a family of their own.

"Da tutti voi mi sono sentito accolto fin dall’inizio. Un grazie con affetto. C’è vediamo all’Elba"

Special thanks go to Rob Paulissen and Willem Schipper. During my time at Thermphos International - as well as the years that followed - we had many fruitful, sometimes fiery discussions. Their input was absolutely invaluable and I dedicate proposition 6 to them. I would also like to thank Rob de Ruiter, Chris Thomas, Peter Geelhoed, Jan Dominicus, Robert Minderhoud, Corrie Autiero, Jan Meijer and the rest of the people at Thermphos International for their (financial and otherwise) support throughout the years.

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Lara, Nelke (my South African-Dutch connection), Gianluca D (a very cool Italian), Diana (an equally cool Columbian), Savad (a great dancer), Phillip (a true Namibian), Phil (my South African connection), Ruth, Francesco M, Fransesco F, Mattia, Gianluca, Stefano, Christiaan (the German), Christian (the Colossus), Elvira, Giampietro, Tamara, Pidio, Yann, John (the sailor), Jacopo (a true thinker and great friend to both of us), Alexi (the climber), Veronica, Gijs (Vrystaat), J@spere, Wilma, Aylin.

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There is a special place for Jacques Eksteen - a great scientist, a great guy, a great inspiration, undoubtedly a great father and someone who gave me a chance. Dankie Jacques! Thanks also to Louise for all her help those first couple of days in The Netherlands.

My IRM colleagues at Corus: Willemijn (the song specialist), Wouter (who saved my skin), Cor (with the beautiful hometown), Maria (my roommate), Alida (I see you!), Elisa (the photo), Erik (the Newcastle rugby fan), Jim (the clever one), Andre (the secret KDRI agent), Martin (the old hand), Jeroen L (and his Irma), Mark H (thanks for your password), Jan (the Feyenoorder - 2 1 op 18 05), Jolanda (the newborn), Tako (my TUDelft connection), Yvette (the 4-day specialist), Frans (another man full of pleasant surprises), Bert (the triathlete), Jeroen S (the musician), Maartje (the fit one), Ronald (who put me on my way), Raymon (his recipe is sublime), Rein (the AZ’er), Christiaan (the Latex king), Bart (the residence permit specialist), Hans H (the Bluenoter), Mark D (the ex-Roland Holstlaan’er), Koen (een Bolletje toch?), Joop (bedankt voor jouw hulp op mijn laaste dag!), Gert-Jan (the vegetarian), Jaap M (the veteran), Jaap B (the G’er), Ron (the ex-flexer), Gerrit (the koke proever), Donald (the analyst), Flip (can I go faster, sure I can), Floor (the TV is big enough, thank you) and Inneke (simply the one).

"Dr. Mostert, ek onthou u vandag helderder as ooit!"

"Juffrou Munro, vandag kom my amptelike opleiding tot ‘n einde. Snaaks dan, dat dit wat tot vandag toe nog vir my die meeste beteken, is my begin!"
Appendix H

Curriculum vitae

Personal
Name: Emile Scheepers
Date of Birth: 5 March 1975
Place of Birth: Somerset West, South Africa

University education

- **April 2003 - May 2007**: Doctoral Researcher (Promovendus) at Delft University of Technology, The Netherlands. The research is carried out as part of a venture involving SenterNovem, Thermphos International and Delft University of Technology.

- **2000 - 2002**: M.Eng.(Extractive Metallurgy) at University of Stellenbosch, South Africa (while working full-time).
  
  *A one-dimensional, quasi-steady state model for the desulphurisation injection process at Saldanha Steel* (now Mittal Steel)

- **December 1998**: Graduated B.Eng.(Chemical Engineering with Metallurgical option), University of Stellenbosch, South Africa.

  Four (one as second author) publications in refereed international journals and eight in international conference proceedings. Co-supervisor of Allert Adema, final year master student.

Working experience

- **May 2007 - present**: Researcher Ironmaking, Corus Ijmuiden, The Netherlands

- **1999 - March 2003**: Technical Officer at the Department of Process Engineering, University of Stellenbosch, South Africa.

Twenty-one point one in 78:24.