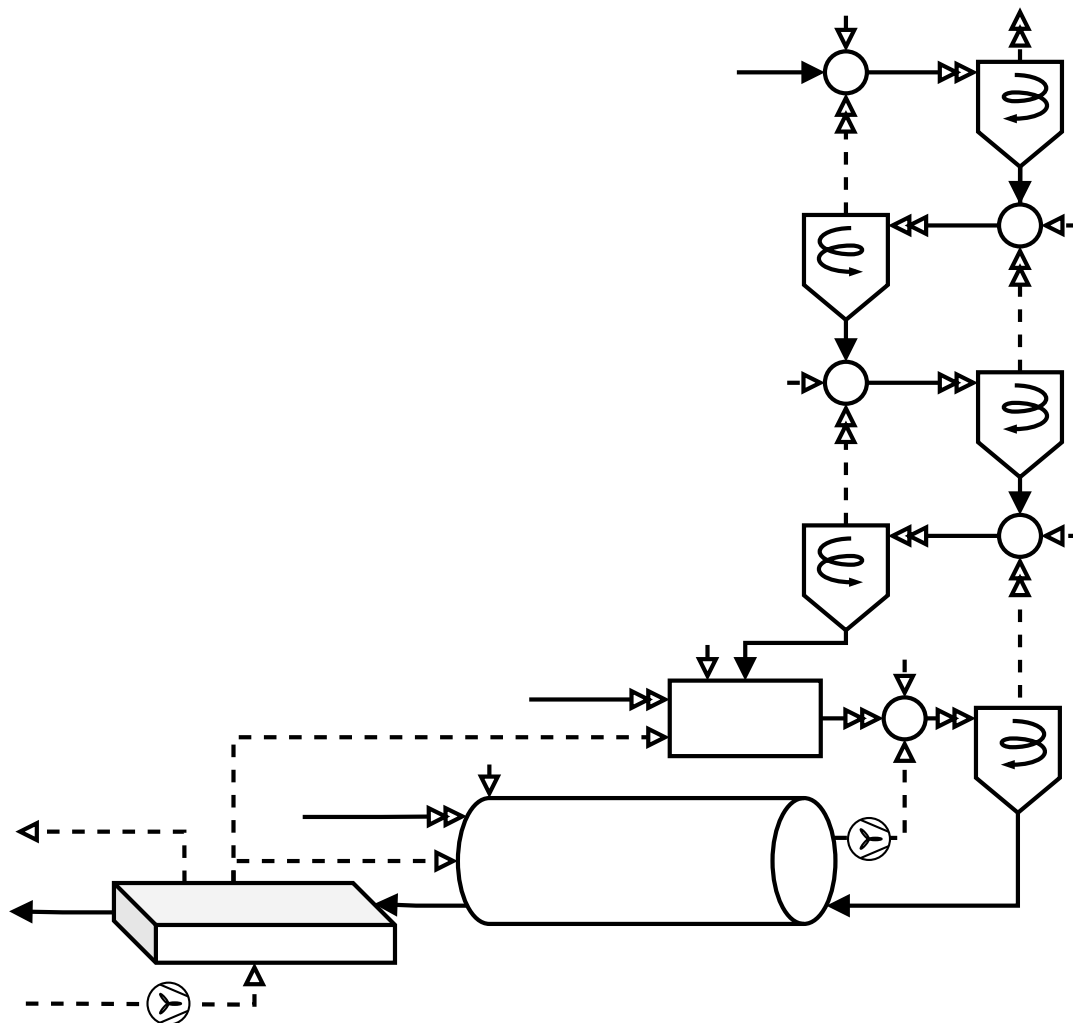




Cement-Process Modelling Towards Electrification

Ground-Up Development of MATLAB Code
Based on Mass and Energy Balances

Master's Thesis in Innovative and Sustainable Chemical Engineering

WILLIAM PALMNÄS

DEPARTMENT OF ENVIRONMENTAL AND ENERGY SCIENCES

CHALMERS UNIVERSITY OF TECHNOLOGY

Gothenburg, Sweden 2026

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Department of Environmental and Energy Sciences
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Supervisors: Alice Fakt, Adrian Gunnarsson & Klas Andersson, Environmental and Energy Sciences

Informants: Marcus Timgren & Bodil Wilhelmsson, Heidelberg Materials

Examiner: Klas Andersson, Environmental and Energy Sciences

Master's Thesis 2026
Department of Environmental and Energy Sciences
Energy Technology
High-Temperature-Processes Group
Chalmers University of Technology
SE-412 96 Gothenburg
Telephone +46 31 772 1000

Cover: An unlabelled flowsheet of the flame-based process with all seven false-air ingresses. Readers are welcome to try and identify the process equipment and the streams.

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ABSTRACT

Developed is the code that solves the solids mass balances from raw meal to clinker, with recirculation and calcination. Solves the Gas mass balances from cooler to preheater, with false air and reactions. Solves the energy balances of the coupled system with non-linear, species-specific thermodynamic properties, and accounting for losses to the surroundings by articulating the complex pieces of equipment from geometrical shapes, for which there are mechanistic and empirical heat-transfer models. Algebraic, ordinary differential, and partial differential equations comprise the heat balances. Solids temperature exiting the rotary kiln was locked at 1450 °C to decouple cooler and tertiary-air pipeline from the calciner, and breaking down the need for phasic heat-transfer phenomena in the rotary kiln. The Cooler was modelled as an elliptic 1-D PDE coupled to a parabolic 1-D PDE. The preheater-calciner-separator tower was modelled as a system of fifteen algebraic equations. The rotary kiln was modelled as a single ODE. Kiln and tower were coupled using the sequential modular method. Results were compiled for a variety of one-by-one adjustments of critical process parameters: False-Air discharge, raw-meal feed, calciner conversion, cyclone separation efficiency, as well as switching to plasma torches. Emergent behaviour, which is the central concept encountered in strongly coupled systems, was expected and prevalent throughout the code. That, from a set of balance equations, emerges a vast network of complexity.

Keywords: MATLAB, coding, modelling, cement production, cement process, plasma, electrification, Heidelberg, energy balance, CO₂ emissions, heat transfer.

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CONTENTS

1	Introduction	1
1.1	Background	1
1.2	Aim	3
1.3	Limitations	3
1.3.1	Calcination Kinetics	3
2	Theory	4
2.1	Cyclone Separator	4
2.2	Mixing	5
2.2.1	Exergy	5
2.3	Heat Transfer	5
2.3.1	Inner Wall	5
	Turbulent Pipe Flow	6
	Rotary Kiln	6
	Cooler Ceiling	6
2.3.2	Wall	6
	Flat Plates	6
	Cylindrical Shells	6
	Truncated Conical Shells	6
2.3.3	Outer Wall	7
	Forced Convection	7
2.3.3.1	Natural Convection	7
	Vertical Plates	8
	Vertical Cylinders	8
	Horizontal Plates	8
	Horizontal Cylinders	8
3	Methodology	9
3.1	Solid-Phase Mass and Species Balances	10
3.1.1	Preheater	11
3.1.2	Recirculation Loop	12
3.2	Gas-Phase Mass and Species Balances	13
3.2.1	False Air	13
3.2.2	Flame	15
3.2.3	Plasma	15
3.3	Energy Balances	16
3.3.1	Lumped Systems	16
3.3.1.1	Preheater	16
3.3.1.2	Calciner	17
3.3.1.3	Separator	18
3.3.2	One-Dimensional Pipe-Flow Systems	18
3.3.2.1	Tertiary-Air Pipeline	18
3.3.2.2	Rotary Kiln	19
	Reducing the order of differential equations	21
3.3.3	Cooler	22

3.3.3.1	Emergence of Composite Heat Loss	23
4	Results	25
4.1	Results of Mass Balances	25
4.2	Results of Heat Balances	26
4.3	Sensitivity Analysis	27
4.3.1	False-Air Effect	27
4.3.2	Raw-Meal-Mass-Flow Effect	28
4.3.3	Plasma	28
4.3.4	Separation-Efficiency Effect	29
4.3.5	Conversion Effect	30
4.4	Differential Equations	31
5	Discussion	33
5.1	Sources of Error	33
5.1.1	Kiln-Hood Location	33
5.1.2	Conversion	33
5.2	Plasma Retrofit	34
5.3	Next-Generation Cement Plant	34
6	Conclusions	35
6.1	Future Modelling Work	35
6.1.1	Rotary-Kiln Upgrades	35
6.1.2	Calcination Kinetics	35
7	Appendix	I

NOMENCLATURE

Constants

α	Phase volume fraction	H	Height of solid bed in the cooler
σ	Stefan-Boltzmann constant	L	Length
ε	Emissivity	W	Width of cooler
M	Molar mass [kg/mol]	X	Characteristic length in cooler
P	Pressure [Pa]	x	Belt direction in the cooler
R_{Air}	Gas constant for air in [J/kg K]	y	Gas-flow direction in the cooler

Dimensionless Numbers

Gr	Grashof number
Nu	Nusselt number
Pe	Péclet number
Pr	Prandtl number
Ra	Rayleigh number
Re	Reynolds number

Functions

μ	Dynamic viscosity [kg/m s]
c_p	Isobaric heat capacity [J/kg K]
H	Specific enthalpy [J/kg]
h	Heat-Transfer coefficient [W/m ² K]
k	Conductivity [W/m K]
Q	Quantity of thermal power [W]

UA	Composite heat-transfer area [W/K]
------	------------------------------------

Geometrical Quantities [m]

D	Diameter
-----	----------

z	Axial coordinate in pipes
-----	---------------------------

Subscripts

∞	Ambient bulk
d	Discharge coefficient
a	Air
f	Film
g	Gas mixture
i	Inner
o	Outer
se	Solids entrained by gas
s	Solid phase
w	Wall
i, j	Counting indices

Variables

$\dot{m}$	Mass flow
-----------	-----------

η	Contextual efficiency
--------	-----------------------

ψ	Entrainment fraction in cyclones
--------	----------------------------------

A, A^{-1}	Equation matrix, and its inverse	w	Weight fraction
G	Superficial mass velocity [kg/m ² s]	X	Conversion of calcination reaction
T	Temperature [K]	Y	CaCO ₃ content in limestone
v	Flow velocity [m/s]		

ABBREVIATIONS

CCFR	Calclner Calcination-reaction-to-Flame power Ratio
CFD	Computational Fluid Dynamics
BVP	Boundary Value Problem
IVP	Initial Value Problem
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation

1 INTRODUCTION

Global cement production comprises seven percent of all anthropogenic emission of carbon dioxide. [1] This emission is partly inherent to the process, by the calcination reaction, and partly caused by the combustion of fuels, as heat must be supplied in the process to reach the required high temperatures. The latter source of emission can be excluded from the process, if an alternative is found to be viable. [2] That being a plasma torch.

It is imperative that such a process is modelled [3], to evaluate the changes in the process when plasma supplants fire as the primary heat source. Also to identify and shore up inefficiencies when modifying existing plants for the fuel switch. By extension, serve as a decision basis for designing future cement plants. This endeavour may eventually give future generations greater ability to expand their infrastructure while using less of their finite resources.

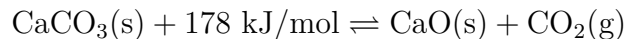
This project concerns the whole cement process, modelling each unit and how they are coupled. A set of MATLAB scripts and functions were developed and results from its calculations are presented and discussed from a mass and energy point of view. Both flame and plasma configurations were also compared.

1.1 BACKGROUND

Modern cities and transportation infrastructure are fundamentally built with concrete [4]. The four primary components of concrete are: cement, water, sand and coarse aggregate. Cement being the binding agent, water makes it flow and set, and aggregates are cheap filler materials that also confer durability. Concrete is useful for its workability, as it can be poured into complex shapes and pumped over distances, and useful for its great strength under compressive loads.

The production of cement begins in a limestone quarry. Where limestone is mined and moved to a crushing plant where it is crushed into fine powder and mixed with sand and clay to obtain desired properties.[4] This raw meal is regarded as the beginning of the process model this work is focused on. The process is depicted in Fig.1.1.

From the solid phase's perspective: The plant begins at the preheater. Which consists of four sequential separation and mixing steps. The purpose of the preheater is to utilise waste heat. The hot meal then enters the calciner where it is further heated to 900 °C by an open flame to spur the endothermic calcination reaction:



Calcined meal is then separated from hot flue gases with a cyclone separator and sent to the rotary kiln, a tilting and rotating furnace, where the meal is further heated by a 2000 °C flame. Wherein a mixture called clinker is formed through a complex reaction series. Immediately as it leaves the kiln (at 1450 °C) – the clinker is rapidly cooled by a fast-moving, ascending flow of air. The process is then concluded. But beyond the cooler is a grinder where gypsum is added, along with other additives, as it is ground into powder, becoming cement. The product may then be stored for a limited time. [4]

Conversely, the gas phase takes a path through the plant that begins at the cooler. Where the cross-flow arrangement heats the air stream unevenly, so to take advantage the higher temperatures it is split into two outlets: Through the hot cooler outlet goes secondary and tertiary air, while the least warm air is vented since it does not contain enough exergy to provide heat anywhere, an example of inherent waste. Secondary air is supplied to the flame-side of the rotary kiln along with cold primary air used to suspend the solid fuels consisting of coal and shredded waste matter. Tertiary air is bypassed the kiln and fed to the calciner. Once deoxygenated these two gas streams are mixed in the separator. And mixed gas cools off as it passes through the cyclones of the preheater, finally expelled from the modelled process. Beyond which, scrubbers remove toxic compounds left in the wake of burning the dirty fuels. Note that Fig.1.1 does an exceedingly poor job of showing where the kiln gas is transferred to. But that is made clear in chapter 3 Methodology.

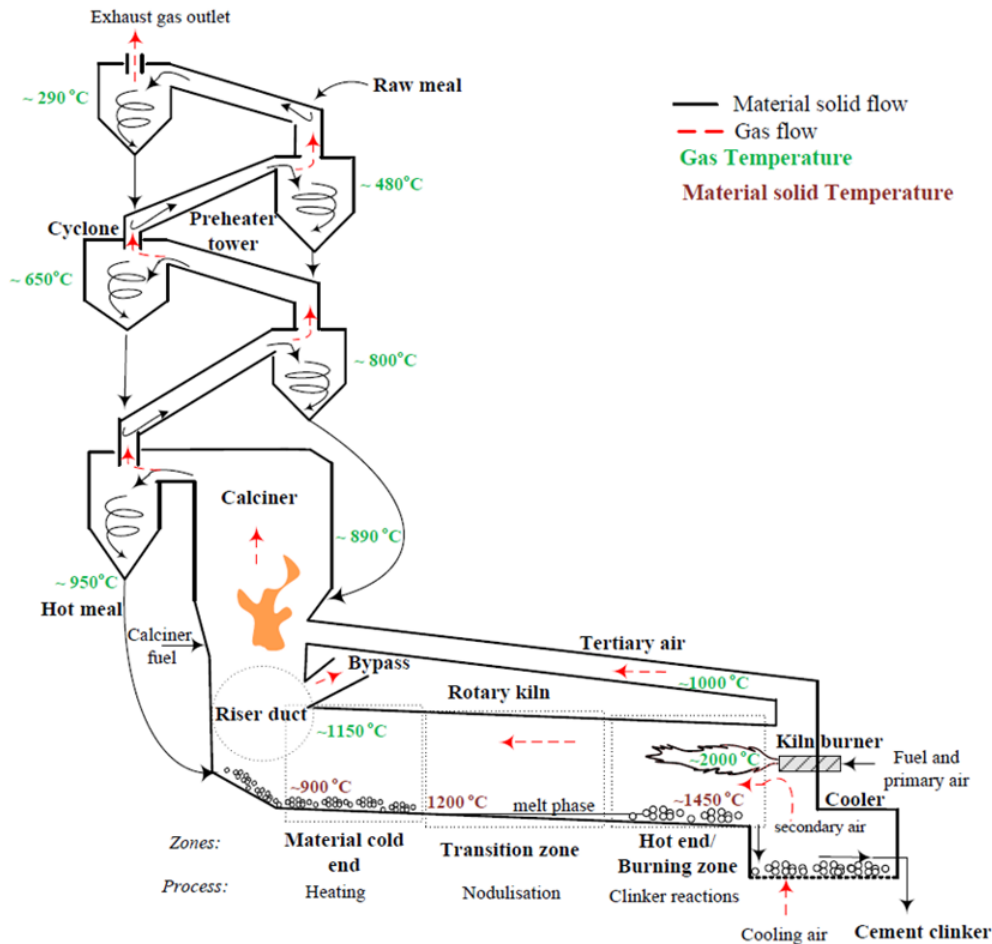


Figure 1.1: Traditional flowsheet of the process. The displayed temperatures are what may be expected from a general process, not necessarily the one on Gotland.

Great difficulty in modelling arises from counter-current action, it increases the strength of coupling between the equations and blurs the concept of a beginning to the solution algorithm; this is emergence[5]. As opposed to a model with strictly sequential coupling - where one balance equation's outputs, are another's inputs, and so on until the end. Such a model (system of equations), are very easy to solve in that they need no initial guess nor outer iterations to achieve convergence.

1.2 AIM

The aim of this master-thesis work was to devise a process model, based on solving heat and mass balances, and translating mathematical models into MATLAB code. The goal is to have the code assist the user who is evaluating different process parameters, by solving for designated output parameters. Research questions posed to the finished work are:

- How does particle-entrainment loss affect cement production?
- What are the heat losses of each unit, and how do they scale with temperature?
- What are the process-level consequences of a fuel switch?
- What emergence do either system possess (flame and plasma)?

1.3 LIMITATIONS

The project does not involve Computational Fluid Dynamics (CFD). The process was exclusively solved in steady state. Some physical descriptions were simplified for the sake of time, code readability, and allowing unimportant phenomena to be decoupled. Many concepts were included to a point of diminishing returns in accuracy; equipment-sizing parameters gave way to great uncertainty. Decoupling is a powerful tool for simplification and is often done to turn an otherwise buggy mess into a robust series of code blocks that may be individually verified for physical plausibility.

The program could not be a general-purpose flowsheet software such as Aspen HYSYS. Where the user selects any process parameter as input and have it automatically solve for the rest. It also was not built with such software, as it would not have the same potential for expansion and customisation as scripting did. Future projects and master theses may be built upon this very code.

1.3.1 CALCINATION KINETICS

Given that electrification will radically increase the partial pressure of CO_2 (discussed under 3.2.3), and given that a high partial pressure of CO_2 in the calciner will shift the equilibrium reaction to yield less CaO , requiring hotter temperatures for the same conversion. [6] So the process model that aspires to capture the effects of electrification would ideally support chemical reaction physics. But alas, extensive literature studies indicate that this goal lies beyond the scope of the project. [7]

Thus, a short cut can be taken by directly providing a reasonable value for calciner conversion X . For example, too large conversion and the calciner runs too cold rendering the specified conversion implausible. The uncertainty in X is matched by the uncertainty in particle size distribution, which is mechanistically tied to X .

To help keep a reasonable temperature in the calciner across a wide range of inputs without manual intervention. A ratio between the heat sink and heat source was introduced (Eq.1.1). With it, conversion may be obtained from solid-phase mass balances 3.1

$$\text{CCFR} = \frac{Q_{\text{Calciner}}^{\text{Calcination}}}{Q_{\text{Calciner}}^{\text{Flame}}} \quad (1.1)$$

2 THEORY

The most important concepts – to recognise before reading the methodology and results of the work – are heat transfer and chemical-engineering thermodynamics, as well as a little momentum transfer. The work also would not be possible without the application of model-simplification techniques, iterative solvers, and fitting polynomials to data.

2.1 CYCLONE SEPARATOR

The cyclone separator is a device that consists of a barrel, riser, cone, pipe, and inlet duct. Depicted in Fig:2.1. The suspension flows rapidly into the barrel at a slanted angle, such that swirling flow is induced. The particles' inertia keep them sliding/rolling along the wall, and falling down the cone where they are funnelled into a narrow pipe. While the gas is sucked out through the riser, located in the eye (centre) of the cyclone (swirl). Hence the name. The ease of separation is modelled as an efficiency factor η . Many intricate

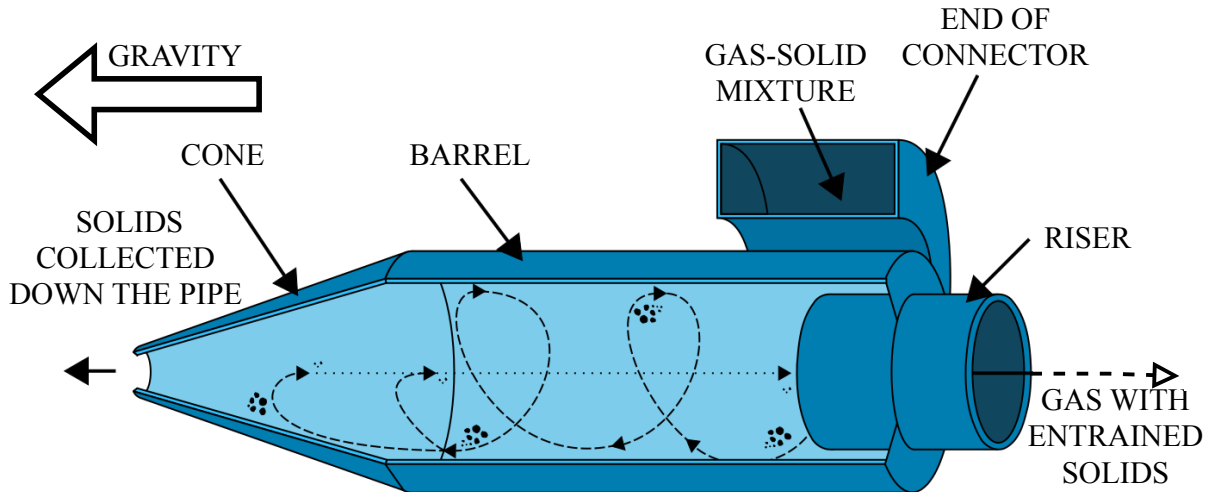


Figure 2.1: Cyclone separator. Note that gravity pulling the particles down the cone is an essential force that makes the separator work. Source: [8].

concepts of fluid dynamics go into the efficiency factor, such as temperature, particle-size distribution, fan power, et cetera. None of which is modelled in the code. The engineers simply provided reasonable efficiencies for each cyclone in the process. And they were kept constant.

Further, the reason why there are four sequentially connected cyclones according to the flowsheet 1.1, is because it allows for counter-current heat exchange to occur in a global sense, while consisting of locally co-current steps. There are three reasons for using co-current heat exchange at all lies in the prevailing multiphase conditions:

1. Vast quantities of pure powder do not flow through heat exchangers
2. Mixing phases together is the fastest way to transfer heat (albeit, with co-current action)
3. Particle-Gas suspensions are cheap to separate (unlike gas-gas, solid-solid suspensions)

2.2 MIXING

Mixing two different fluids (indices 1 and 2) at different temperatures (T_1 and T_2) is equivalent to co-current heat exchange, in that exergy is readily destroyed. Solving for the outlet temperature is possible by solving the non-linear equation given by.

$$0 = Q_1(T_1) + Q_2(T_2) - Q_1(T_{\text{out}}) - Q_2(T_{\text{out}})$$

Given that the powers Q_1 and Q_2 [W] are some polynomial functions of temperature, method of extraction is shown in 7.

2.2.1 EXERGY

Exergy (or energy-cascade concept) is the key aspect of the engineering decisions concerning the gas phase. Recall that counter-current heat exchange is optimal. Because the hot stream only transfers heat to the cold stream when they are simultaneously at their hottest, hot-in and cold-out. Similarly, the solid phase runs counter to the gas phase.

2.3 HEAT TRANSFER

Each piece of equipment will suffer heat losses due to a combination of the three different heat-transfer mechanisms - which are: conduction inside the wall, convection and radiation together on both inner and outer surfaces. The combined interaction is to be calculated for each set of dimensions, materials, and flow characteristics within and without. The essence of composite heat transfer is that thermal resistances are summed, so if the inner+outer resistance is 1/1000 the size of the wall, the small resistances can be neglected and a good model for the wall resistance will very accurately predict the composite heat loss. The method for implementing these phenomena is laid out under section 3.3.3.1. All convective heat-transfer correlations are borrowed from this book[9].

2.3.1 INNER WALL

The inner surface was the hardest to quantify and the least resistive. Firstly due to the multiphase fluid dynamics, mixture properties, reactions that reign inside the process equipment. Secondly, preliminary studies assuming single-phase Nusselt correlations and air properties revealed a lower bound for each heat-transfer coefficient that would be typical for cyclone, pipe and kiln. The lower bounds were consistently found to overpower the conduction rate. Thereby the internal bulk temperature was almost exactly equal to the inner surface temperature. However, the code that draws this conclusion remains in use, to protect against unforeseen consequences of future changes. As per the principle of Chesterton's fence.

Internal gas-wall radiation could be safely neglected, as the gas emissivity is too esoteric for this project, and a model for inner convection was already deemed superfluous. Eqs.2.1 gives the Reynolds number and universal gas-conductivity approximation that are used in the only relevant Nusselt correlation Eqs:2.2 to calculate the inner convective heat-transfer resistance R_{Inner} from Eq.2.1.

$$\text{Re}_i = \frac{4\dot{m}}{\pi\mu D_{wi}} \quad k = k_{\text{Flue-Gas Mixture}} \approx k_{\text{Air}} \quad R_{\text{Inner}} = \frac{1}{\pi L k \text{Nu}_i} \quad (2.1)$$

Turbulent Pipe Flow Dittus and Boelter are credited for this correlation where a fluid being cooled by its surroundings.

$$\boxed{\text{Nu}_i = 0.023 \text{Re}_i^{0.8} \text{Pr}^{0.3}} \quad \text{Re}_i > 10^4 \quad \text{Pr} \in (0.7, 100) \quad L/D_{\text{wi}} > 60 \quad (2.2)$$

The last constraint is stipulated by Dittus and Boelter because fully-developed flow was used in their experiments. But this will be violated and it won't matter since inner resistance is so small. Giving any halfway decent description of inner convection is already going above and beyond.

Rotary Kiln is explained thoroughly in the same paper that provided the other kiln-related models. [10]. Wherein it is labelled *gas-wall convection*.

Cooler Ceiling is exclusively described as radiation since convection is already accounted for in the bed, and this heat loss term only applies to the solids top boundary.

$$R_{\text{Inner}} = \frac{1}{\sigma \varepsilon_{\text{wi}} (T_s + T_{\text{wi}}) (T_s^2 - T_{\text{wi}}^2) W L}$$

This model fails to capture the smoothening effect of diffraction and view factors to upstream and downstream portions of the surfaces, which is no great loss of accuracy as the distance between the bed and the ceiling is unknown. As well as they pale in comparison to the devastating scarcity of HEIDELBERG information regarding the cooler.

2.3.2 WALL

The wall is dominated by conduction, since we may regard the wall materials as opaque to all wavelengths of photons released by black-body radiation. Conductive resistance is constant and analytically solvable given a temperature-independent conductivity and for simple geometries. Three such geometries are needed to articulate any shape encountered in the process (notably complex are the cyclones with their barrels and cones).

Flat Plates

$$R_{\text{Plate}} = \frac{\delta}{k_{\text{Wall}} A} \quad \text{Single layer} \qquad R_{\text{Plate}} = \sum_j \frac{\delta_j}{k_j A} \quad \text{Multiple layers}$$

Cylindrical Shells

$$R_{\text{Cylinder}} = \frac{\ln(D_{\text{Outer}}/D_{\text{Inner}})}{2\pi L k_{\text{Wall}}} \quad D_{j+1} = D_j + 2\delta_j \quad R_{\text{Cylinder}} = \sum_j \frac{\ln(D_{j+1}/D_j)}{2\pi L k_j}$$

Cumulative sum

Truncated Conical Shells are a part of the cyclone separators, very difficult. The geometry in question is illustrated in Fig.2.2. With radii r , resistance R , height of cone section H , cone-tilt angle α , wall thickness δ . Starred quantities are dimensionless.

$$\tan(\alpha) = \frac{r_t - r_b}{H} \quad r_b^* = \frac{r_b}{H} \quad z_b^* = \frac{r_b^*}{\tan(\alpha)} \quad \tilde{\delta}^* = \frac{\delta \cos(\alpha)}{H}$$

$$R_{\text{Cone}} = \left(2\pi k H \int_{z_b^*}^{z_b^{*+1}} \left(\ln \left(\frac{r_b^* + (z^* - z_b^*) \tan(\alpha) + \tilde{\delta}^*}{r_b^* + (z^* - z_b^*) \tan(\alpha)} \right) \right)^{-1} dz^* \right)^{-1} \quad (2.3)$$

Equation 2.3, as written, only accounts for the case of a single layer. How one would deal with multiple layers is left to the imagination of the reader.

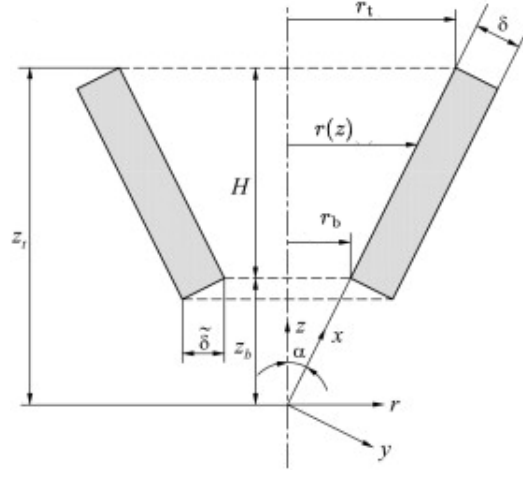


Figure 2.2: Conical sections in the cyclones, diagram and method was taken from [11].

2.3.3 OUTER WALL

Both convection and radiation will be modelled on the outer surface, as per:

$$R_{\text{Outer}} = \frac{1}{\underbrace{\frac{k_a \text{Nu}_o}{D_o}}_{\text{Convection}} A_o + \underbrace{\sigma \varepsilon_o (T_{\text{wo}} + T_\infty) (T_{\text{wo}}^2 - T_\infty^2)}_{\text{Radiation}} A_o}$$

However, there are two distinct phenomena that govern the rate of convective heat transfer. Forced convection (sometimes referred to as advection) and natural convection.

Forced Convection is driven by external forces such as wind against the wall, or by rotation ω [1/s] of the kiln wall.

$$\boxed{\text{Nu}_o = \begin{cases} 0.027 \text{Re}_o^{0.805} \text{Pr}^{1/3} & 4,000 \leq \text{Re}_o < 40,000 \\ 0.193 \text{Re}_o^{0.618} \text{Pr}^{1/3} & 40,000 \leq \text{Re}_o < 400,000 \end{cases}} \quad \text{Re}_o = \frac{v_{\text{Wind}} D_{\text{wo}} P_\infty}{\mu_a R_{\text{Air}} T_{\text{fo}}}$$

However, natural convection could supplant it as the dominant mechanism. Therefore the model must check that $\text{Re}^2 > \text{Gr}$. Otherwise it must swap to a Nusselt correlation of Grashof or Rayleigh numbers.

2.3.3.1 NATURAL CONVECTION

Natural convection is buoyancy-driven flow which emerges from the thermal expansion of fluids under a temperature gradient. Wind is regarded as an external force on a given object, but the wind is itself the manifestation of natural convection on planetary scale. The preheater, calciner, and separator are inside a building which provides protection from the wind, but is also assumed not to offer an elevated ambient temperature. So, natural convection is dominant there.

$$\text{Ra}_L = \text{Gr}_L \text{Pr} \quad \text{Gr}_L = B L^3 |T_{\text{wo}} - T_\infty| \quad B := \frac{g \beta}{\nu^2} \quad (2.4)$$

Where B is a function of the outer film temperature and is a mishmash of all the material properties that describe the visco-buoyant forces that cause natural convection to occur. Data was taken for air from this book of transfer[9], and a polynomial was fit for $T \in [288, 480]$ kelvin.

Vertical Plates

$$\boxed{\text{Nu}_L = \left(0.825 + \frac{0.387\text{Ra}_L^{1/6}}{\left(1 + \left(\frac{0.492}{\text{Pr}} \right)^{9/16} \right)^{8/27}} \right)^2} \quad L := \text{Height} \quad \forall \text{Ra}_L \in (0, 1\text{e}13)$$

Vertical Cylinders are the same as vertical plates if curvature effects are small

$$\frac{D_{\text{wo}}}{L} \geq \frac{35}{\text{Gr}_L^{1/4}}$$

Horizontal Plates when the hot surface is facing up, is described by:

$$\boxed{\text{Nu}_L = 0.14\text{Ra}_L^{1/3}} \quad \text{with temporary definition } L := \frac{\text{Plate Area}}{\text{Plate Perimeter}} \quad \forall \text{Ra}_L \in (2\text{e}7, 3\text{e}10)$$

Horizontal Cylinders long enough to have negligible end effects:

$$\boxed{\text{Nu}_D = \left(0.60 + \frac{0.387\text{Ra}_D^{1/6}}{\left(1 + \left(\frac{0.559}{\text{Pr}} \right)^{9/16} \right)^{8/27}} \right)^2} \quad \forall \text{Ra}_D \in (1\text{e-}5, 1\text{e}12)$$

3 METHODOLOGY

The most salient mathematics in the underlying code is presented and discussed. Modelling decisions, approximations, and omissions are stated and justified with help of literature and calculations.

Prior research in the field of cement-process modelling was studied to glean relevant equation-parameter-variable formulations. Those formulations were then modified to fit the specific needs of the process; to account for additional complexities. The equations were compiled and variables were renamed to give a decently consistent notation. The mathematical models were then translated into symbolic expressions in the setup script, and finally used to generate brutally optimised MATLAB functions (denoted as equations). The sequential modular method was used when the solved solids-effluent temperature of the separator was transferred to rotary kiln, letting it solve for its gas-effluent temperature. Which was in turn transferred to the cyclone tower. Looping to convergence, usually taking four iterations to achieve > 1 K difference between current and previous states. Shown in Fig.3.1.

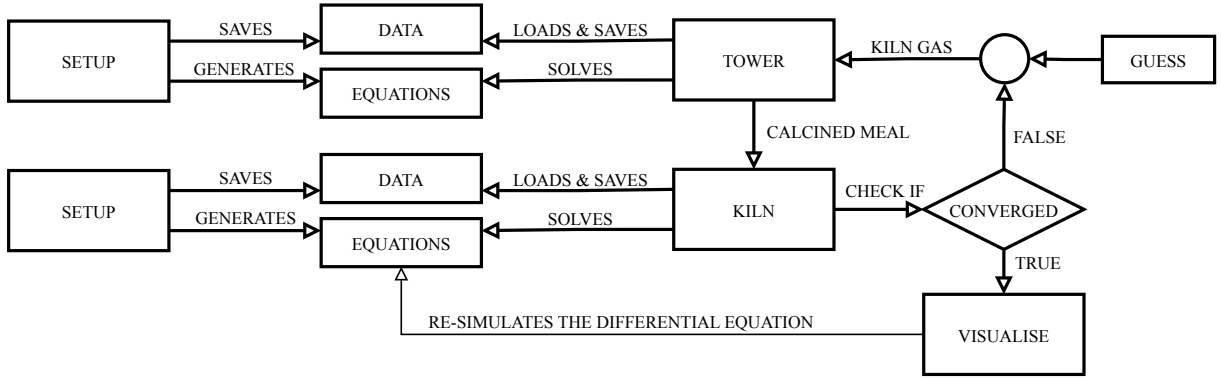


Figure 3.1: Algorithm for coupling the system of algebraic equations (consisting of pre-heater, calciner and separator, its effluent being calcined meal), to the differential equation (kiln, effluent kiln gas) by using the sequential modular method.

The units relate to one other according to the Fig.3.3. Each unit provides the following outputs:

- Mass flows $\dot{m}$
- Molecular weight fractions w_j for both phases
- Temperatures T
- Heat losses $UA \cdot (T - T_\infty)$



Figure 3.2: Arrow-style designation scheme for all diagrams henceforth.

Parameters such as: Incoming mass flows, material compositions, flame powers, pressures, and target temperatures were obtained from an internal heat-balance report. Where the

2022 measurements were used. Marcus Timgren, engineer at Heidelberg Materials, also helped with clarifying how the machinery worked and that the walls of the cyclones had about 20 cm of refractory. Preliminary models, parameters and material properties were borrowed from this [3] stacked cement-process-modelling paper. But the few parameters that could not be found were set according to the intuition of yours truly and supervisors. Which was partly based on experience of running the code itself. But no data-driven methods were used as those would undermine the validity of the model when used to investigate electrification. Data from the cement plant is used to validate the model of the flame-powered process.

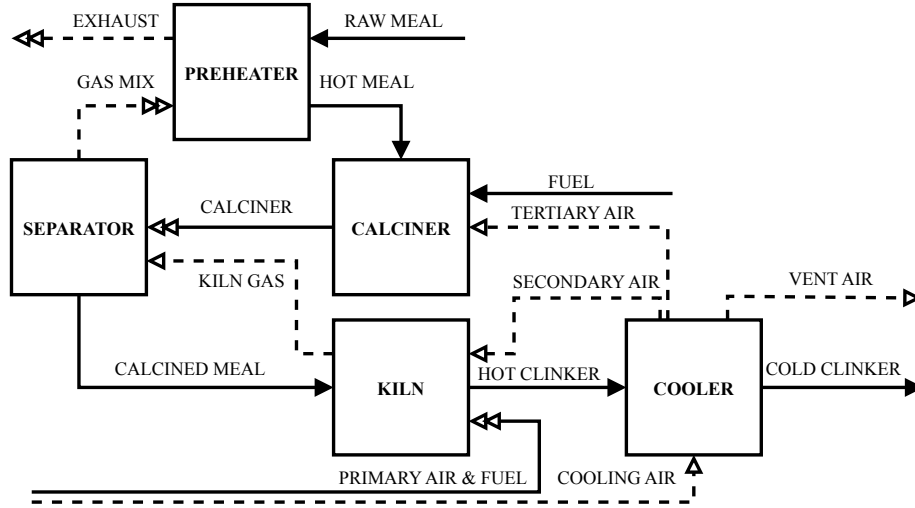


Figure 3.3: Diagram for the main process steps and how they are connected. The preheater is considered the sum of four cyclone step.

The code is written in standard SI units, meter, second, kilogram, pascal, kelvin, mole, joule, and so on. If an alternative unit (such as celsius or bar) is requested then unit conversions will be applied to the input and the output.

3.1 SOLID-PHASE MASS AND SPECIES BALANCES

Five solid species were accounted for CaCO_3 , CaO , Fe_2O_3 , SiO_2 , and Al_2O_3 . Raw limestone was assigned a purity $Y = w_{\text{CaCO}_3}^{\text{Raw Meal}}$, and then the proportions of the other species were set. Table 3.1 shows the incoming material compositions. Whereas table 4.1 also shows the output compositions.

Table 3.1: Five species, where the last three are considered inert to the modelling effort, and their only purpose is to give realistic enthalpies to the energy balances.

	w [%]				
	CaCO_3	CaO	SiO_2	Fe_2O_3	Al_2O_3
Ash	0	0	80	10	10
Raw Meal	75	0	15	7	3

3.1.1 PREHEATER

The preheater consists of four cyclone separators, coupled according to Fig.3.4. The reason for this is to maximise exergy efficiency, which is discussed in section 2.2.1. The

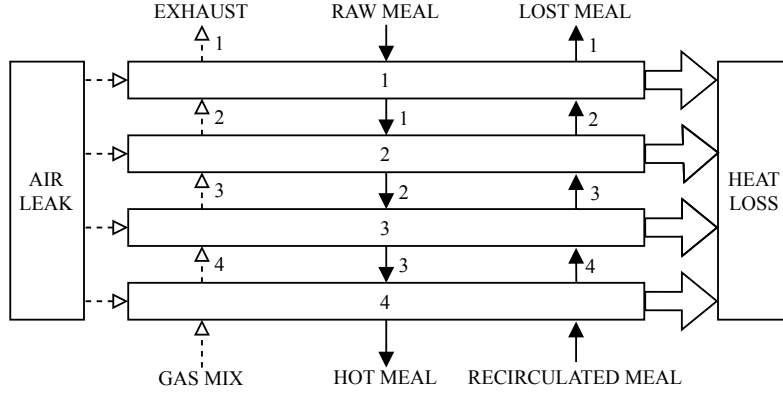


Figure 3.4: The diagram shows how the phases move between the cyclones, the air leaking in due to suction, as well as the heat loss to the environment.

solid-phase mass balance of over the preheater consists of a set of local mass balances over each cyclone. Which in turn are set up by imposing steady-state operation upon the i :th cyclone. Which is done as follows: the mass flow of solids entering from above $\dot{m}_{i-1}^s$ and the mass flow of entrained solids entering from below $\dot{m}_{i+1}^{se}$ is equal to the total outgoing solids from the cyclone in question $\dot{m}_i^s + \dot{m}_i^{se}$. [3]

$$\dot{m}_{i-1}^s + \dot{m}_{i+1}^{se} = \dot{m}_i^s + \dot{m}_i^{se} \quad (3.1)$$

The problem with this equation is that it has two unknown mass flows per cyclone, to make the system of linear equations solvable the mass flow of entrained solids must be substituted with a linear equation of the collected-solids mass flow.

$$\dot{m}_i^{se} = \psi_i \dot{m}_i^s \quad (3.2)$$

The cyclones are not able to perfectly separate solids from gas, thus the entrained solids that follow the ascending gas are taken into account through the use of a separation-efficiency factor $\eta := \frac{\text{Collected}}{\text{Inflow}}$. It is the traditional formulation in the field of cyclone separation, because it is the most intuitive. But Eq.3.2 is needed here. So the code takes user-specified values η_i (one for each cyclone), then uses Eq.3.3 to convert η to ψ . Where $\psi := \frac{\text{Entrained}}{\text{Collected}}$.

$$\psi_i = \frac{1}{\frac{1}{1 - \eta_i} - 1} \quad (3.3)$$

The full system of linear algebraic equations can be shown specifically for a four-step preheater (equations 3.4-3.7), by applying the external inflows at the top and bottom cyclones according the Fig.3.4. Before substituting Eq.3.2 into 3.1.

$$(1 + \psi_1)\dot{m}_1^s = \dot{m}_{\text{Raw Meal}} + \psi_2\dot{m}_2^s \quad (3.4)$$

$$(1 + \psi_2)\dot{m}_2^s = \dot{m}_1^s + \psi_3\dot{m}_3^s \quad (3.5)$$

$$(1 + \psi_3)\dot{m}_3^s = \dot{m}_2^s + \psi_4\dot{m}_4^s \quad (3.6)$$

$$(1 + \psi_4)\dot{m}_4^s = \dot{m}_3^s + \dot{m}_{\text{Separator}}^{se} \quad (3.7)$$

Equations 3.4-3.7 can be expressed as one matrix equation 3.8. Which is $Ax = b$ on standard form, The matrix A may then be inverted A^{-1} so that the unknown variable vector x can be calculated directly according to $x = A^{-1}b$.

$$\begin{bmatrix} 1 + \psi_1 & -\psi_2 & 0 & 0 \\ -1 & 1 + \psi_2 & -\psi_3 & 0 \\ 0 & -1 & 1 + \psi_3 & -\psi_4 \\ 0 & 0 & -1 & 1 + \psi_4 \end{bmatrix} \begin{bmatrix} \dot{m}_1^s \\ \dot{m}_2^s \\ \dot{m}_3^s \\ \dot{m}_4^s \end{bmatrix} = \begin{bmatrix} \dot{m}_{\text{Raw Meal}} \\ 0 \\ 0 \\ \dot{m}_{\text{Separator}}^{\text{se}} \end{bmatrix} \quad (3.8)$$

Equation Matrix: A Unknown: x Known: b

Thus, the mass flow rate of the j :th species that is collected by the i :th cyclone $\dot{m}_{ij}^s$ can be calculated according to Eq.3.9. It involves the first and last columns of the inverted matrix A , named $F_i = \{A^{-1}\}_{i,1}$ and $L_i = \{A^{-1}\}_{i,4}$ respectively.

$$\dot{m}_{ij}^s = F_i \dot{m}_j^{\text{Raw Meal}} + L_i \dot{m}_j^{\text{Recirculated Meal}} \quad (3.9)$$

This approach was invaluable when sorting out the recirculation loop, because only two columns in the inverted matrix were relevant. Without the use of matrix inversion, an iterative method would be required, which would only add complexity and confusion.

3.1.2 RECIRCULATION LOOP

There is a recirculation loop between the preheater, calciner and separator where partially calcined meal particles are re-exposed to the flame in the calciner. This requires another layer of modelling. The behaviour is accounted for by setting up and solving linear equations using the flow rates of each species of the entrained solids from the separator $\dot{m}_j^{\text{Recirculated}}$.

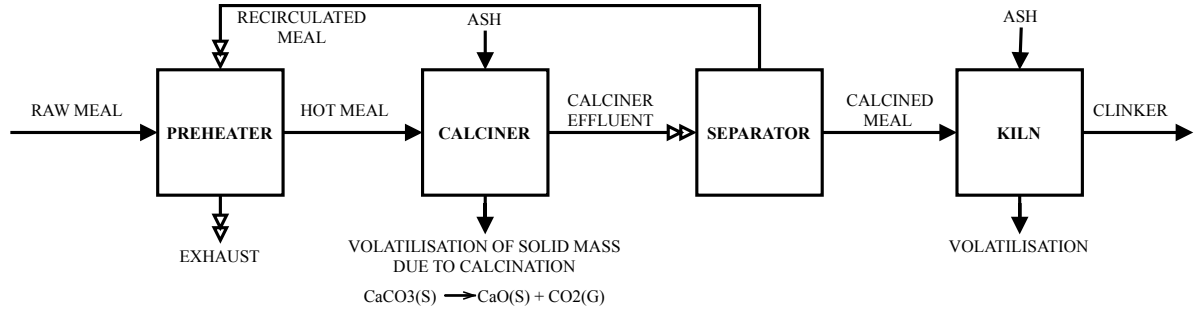


Figure 3.5: Diagram of the process concerning the solids mass balance. Recirculated-Meal stream is named 'Gas Mix' in the gas-balance perspective (next section). The names calciner effluent and calciner have no semantic difference.

The system of equations 3.10-3.12 is the general formulation that works well for all inert species, (all species j whose mass reaction rates $\dot{m}_j^{\text{Reaction}} = 0$). The left-hand side of each implicit equation is always arranged to be zero. In this particular section, implicit equations are analytically solvable using `solve` (symbolic rearrangement).

$$\dot{m}_j^{\text{Hot Meal}} = F_4 \dot{m}_j^{\text{Raw Meal}} + L_4 \dot{m}_j^{\text{Recirc}} \quad (3.10)$$

$$\dot{m}_j^{\text{Calciner}} = \dot{m}_j^{\text{Hot Meal}} + \dot{m}_j^{\text{Ash}} - \dot{m}_j^{\text{Reaction}} \quad (3.11)$$

$$0 = \dot{m}_j^{\text{Recirc}} - (1 - \eta_{\text{Separator}}) \dot{m}_j^{\text{Calciner}} \quad (3.12)$$

Whereas, CaCO_3 and CaO balances (Eqs.3.13-3.15) are formulated individually, but derived from the general system Eqs.3.10-3.12. Where the mass reaction rates were substituted for a conversion ratio X .

$$0 = \dot{m}_{\text{CaCO}_3}^{\text{Recirc}} - (1 - \eta_{\text{Separator}})(1 - X)\dot{m}_{\text{CaCO}_3}^{\text{Hot Meal}} \quad (3.13)$$

$$0 = X - \frac{Q_{\text{Flame}}^{\text{Calcliner}} M_{\text{CaCO}_3}}{\dot{m}_{\text{CaCO}_3}^{\text{Hot Meal}} \Delta H_{\text{Calcination}}} \times \text{CCFR} \quad (3.14)$$

$$0 = \dot{m}_{\text{CaO}}^{\text{Recirc}} - (1 - \eta_{\text{Separator}}) \left[X M_{\text{CaO}} \frac{\dot{m}_{\text{CaCO}_3}^{\text{Hot Meal}}}{M_{\text{CaCO}_3}} + \dot{m}_{\text{CaO}}^{\text{Hot Meal}} \right] \quad (3.15)$$

3.2 GAS-PHASE MASS AND SPECIES BALANCES

Once the solids mass balance has been solved, the mass flow rate of clinker entering the cooler has been uncovered. And that 1450- °C clinker must be cooled with a proportionally heavy air stream, composition shown in table 3.2. The target temperature for the cooled clinker is around 100 °C. Therefore we specify four proportional air flows: Primary, secondary, tertiary, and vent air. Confer with the Fig.3.6, to see how they are coupled with the process. Note that recirculation of gas is not modelled, since it is only a miniscule

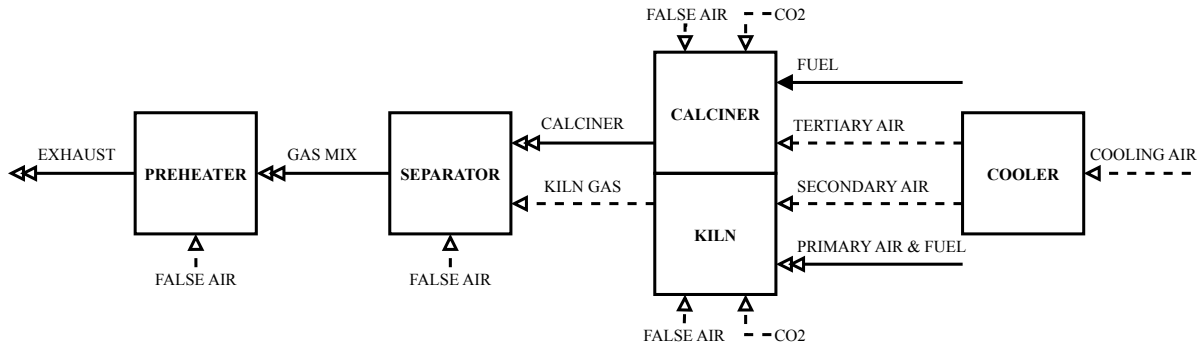


Figure 3.6: The process from the gas' perspective. The false air coming in to the preheater and separator is especially undesired. Calciner false air is needed for combustion. The CO_2 entering the reactors comes from volatilisation.

trickle of gas that fills the void space between the collected solid particles. This effect is provably small by the phasic density ratio $\rho_g/\rho_s < 0.001$.

Table 3.2: Air composition. Dry air was assumed for all tests.

	w [%]						
	N_2	O_2	Ar	CO_2	H_2O	HCl	SO_2
Air	75.51	23.14	1.28	0.06	0	0	0

3.2.1 FALSE AIR

False or undesired air enters each cyclone i because of suction and gaps in the construction. The mass flow rates $\dot{m}_i^{\text{Air}}$ [kg/s] depends on the gauge pressures $P_i < 0$ [kg/m s²], gap areas A_i^{Gaps} [m²], air densities ρ_i [kg/m³], and a discharge coefficient $C_d = (1 + K)^{-1/2}$ - (boxed Eq.3.17). Which is an empirical parameter that quantifies the energy losses that the flow suffers when traversing the gap ($C_d = 1$ being perfectly lossless). To solve this fluid-dynamics problem, Bernoulli's equation and continuity is used. Bernoulli's equation

3.16 is an energy balance involving only mechanical energies, in this case gravitational potential energy is negligible leaving only pressure and kinetic energy. It is also assumed that the energy loss occurs suddenly when the air is so close to the gaps of the vessel such that the air has been warmed to internal bulk temperature.

$$\begin{aligned} P_{\text{Ambient}} + \frac{\rho_1 v_1^2}{2} = P_{\text{Inside}} + \frac{\rho_2 v_2^2}{2} + K \frac{\bar{\rho} \bar{v}^2}{2} \Rightarrow 0 = P_i + \frac{\rho_i (v_i / C_d)^2}{2} \Rightarrow v_i = C_d \sqrt{-2P_i \frac{1}{\rho_i}} \end{aligned} \quad (3.16)$$

The continuity equation holds since the flow is at steady state, and the fluid density ρ_i (evaluated at conditions inside the cyclones) is assumed to follow from ideal gas and incompressible flow, since the ingress velocities v_i should be significantly slower than the speed of sound in air $343 \text{ m/s} \times \sqrt{T_i/300 \text{ K}}$, due to the high temperatures.

$$\rho_i = \frac{P_\infty + P_i}{R_{\text{Air}} T_i} \quad \dot{m}_i^{\text{Air}} = A_i^{\text{Gaps}} \rho_i v_i \xrightarrow{(3.16)} \dot{m}_i^{\text{Air}} = A_i^{\text{Gaps}} C_d \sqrt{-2P_i \frac{P_\infty + P_i}{R_{\text{Air}} T_i}} \quad (3.17)$$

The discharge coefficient can be estimated from empirical correlations of a range of geometries (of nozzles). However the real gaps in the process equipment is unknown. The areas have been inferred by engineers at Heidelberg Materials based on oxygen measurements. However the discharge coefficient, which is coded as a constant scalar parameter for all units, is investigated in the sensitivity analysis. The calculations using Eqs.3.16-3.17, are presented in table 3.3. A second table 3.4 presents calculations of an incorrect kiln-hood placement, which were regrettably used for most experiments presented in chapter 4 Results.

Table 3.3: Kiln hood being correctly placed at the burner end. Calculated for $C_{\text{discharge}} = 0.30$.

Preheater #	T [K]	P [Pa gauge]	ρ_{Air} [kg/m ³]	A_{Gaps} [m ²]	v [m/s]	$\dot{m}_{\text{False Air}}$ [kg/s]
1	681.5	-7320	0.48	0.03655	52.36	0.92
2	866.5	-6670	0.38	0.04288	56.17	0.92
3	937	-4590	0.36	0.04288	47.93	0.74
4	1022	-3410	0.33	0.04288	42.88	0.61
Separator	1173	-2770	0.29	0.04288	41.27	0.52
Kiln Hood	1223	-70	0.29	2.778	6.61	5.3

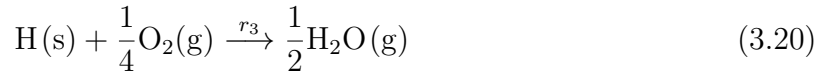
Table 3.4: Measurements for T and P were used as they would be constant, so that obtaining the false-air flows would exclusively depend on the discharge coefficient. Which was chosen to be $C_d = 0.04$ for the base case. Note that a window-size-three moving mean was applied to the gauge-pressure vector, to even out the pressure drops, for an inner heat-transfer correlation which is no longer relevant. The original pressure is in table 3.3.

Preheater #	T [K]	P [Pa gauge]	ρ_{Air} [kg/m ³]	A_{Gaps} [m ²]	v [m/s]	$\dot{m}_{\text{False Air}}$ [kg/s]
1	681.5	-7450	0.480	0.037	7.048	0.124
2	866.5	-6193.333	0.382	0.043	7.198	0.118
3	937	-4890	0.359	0.043	6.606	0.102
4	1022	-3590	0.333	0.043	5.872	0.084
Separator	1173	-2646.667	0.293	0.043	5.376	0.068
Kiln Hood	1223	-2265	0.282	2.778	5.068	3.973

3.2.2 FLAME

Traditional cement production relies on combustion to supply the high-energy-at-high-temperature demand. The fuel mix mostly consists of non-recyclable refuse like shredded tires, plastics, textiles and paper, but also coal. Data exists on the fuels' compositions, feed rates, and lower heating values (disallowing the heat recovery from steam in the exhaust). Which are used to inform the mass and species balances of both phases.

Seven gas species were accounted for, N_2 , O_2 , CO_2 , H_2O , Ar , HCl , and SO_2 . Four complete-combustion reactions (Eq.3.18-3.21) were used. Where r_2 and r_3 compete for the same solid hydrogen, but r_2 is assumed to 'go first', and somewhat deplete the available hydrogen for r_3 to form water.



3.2.3 PLASMA

Plasma torches can power the calciner and rotary kiln without oxygen. The process does still require some amount of gas flow to enable waste-heat utilisation. The volatilised CO_2 is recirculated along with false air by connecting the preheater's exhaust to the clinker cooler, with a gas cooler and in between, Fig.3.8.

The mass flow rates of secondary- and tertiary-gas are still independent parameters, because it is a steady-state, closed-loop system. The vent-gas flow must balance with the total incoming mass flow from volatilisation and from false air, depicted in Fig.3.7 and expressed as Eq.3.22. The gas composition of the j :th species in the vent is calculated from the weighted mean Eq.3.23.

$$\dot{m}_{Vent} = \dot{m}_{Calciner}^{CO_2} + \dot{m}_{Kiln}^{CO_2} + \dot{m}_{False\ Air} \quad (3.22)$$

$$w_j^{Vent} = \frac{(\dot{m}_{CO_2}^{Calciner} + \dot{m}_{CO_2}^{Kiln} + \dot{m}_{False\ Air} w_j^{Air})}{\dot{m}_{Vent}} \quad (3.23)$$

The gas composition (j :th species' mass fraction w_j^{Vent}) will be constant across the tertiary pipeline and for most of the kiln. Then CO_2 is added in the calciner and in the kiln. Those streams are then mixed and brought to the separator and preheater wherein false air is added. The j :th species' mass flow is assumed to be calculated in each step along the process to inform the heat balances of the correct enthalpy functions 3.3.1.

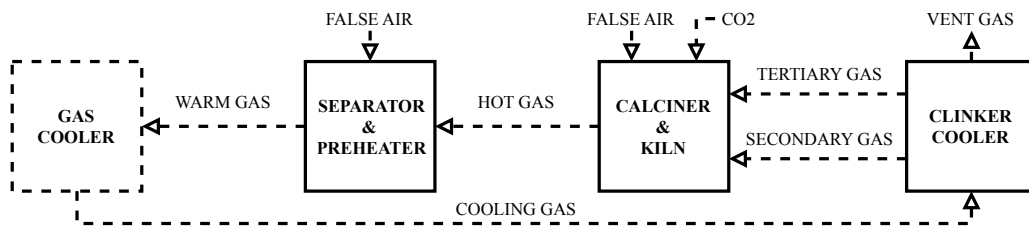


Figure 3.7: Plasma process from the gases' perspective. The exhaust stream in the flame-powered process was renamed to warm gas.

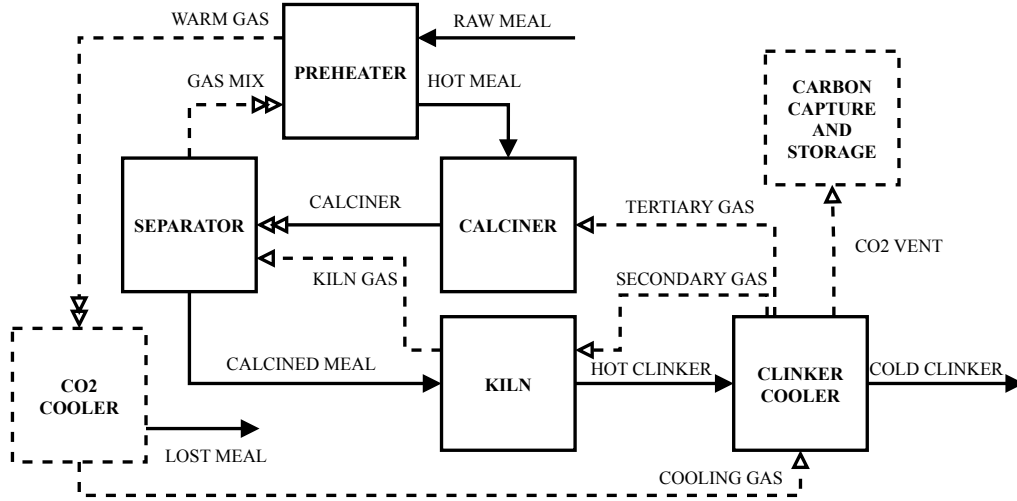


Figure 3.8: Plasma process has gas recirculation and less overall gas mass flow.

3.3 ENERGY BALANCES

The final major step is to obtain the stream temperatures and heat losses over each unit. It is much more difficult to model heat transfer and energy balances than it is to set up and solve mass balances, because it requires many non-linear material properties. The composite heat-transfer areas $UA_{\text{Calciner}}^{\text{Mixing}}$ governing the rate of cooling is obtained from the methods presented in section 2.3: Inner wall: Negligible, conduction through cylindrical shells, forced external convection across horizontal cylinders.

3.3.1 LUMPED SYSTEMS

Lumped systems are considered to be perfectly mixed, thereby modelled with algebraic balance equations, rather than differential equations. Lumping is only done for fast-moving, turbulent, highly three-dimensional, multiphase flows. Without the act of lumping, the goal of this master thesis would be unachievable, because CFD would be needed, which is not a good tool for running such a large number of units. Anyway, these algebraic balance equations have incoming and outgoing powers Q . Formulated as polynomial functions of temperature T , based on the mass-flow mixtures, which were obtained by solving all mass balances beforehand. The polynomials are made by using `polyfit` on a few temperature values by calculating the enthalpies for any given mixture of species, using the complete functions for each individual specie. This process is explained in the appendix, 7 enthalpy. The subscripts are used to identify streams, when building the system of equations the units themselves are not in need of identification, rather it is the effluent streams from each unit that are useful. Therefore Q_{Calciner} refers to the heat flow of the gas and solids leaving the calciner.

3.3.1.1 PREHEATER

The preheater consists of ten cyclone separators forming a series of four steps, coupled in such a way as to mix warm particles from above with hot gas rising from below, before separating them again to funnel the particles down into increasingly hotter cyclones. Numbered indices (1-4) are reserved for the preheating cyclones. Equations 3.24-3.27 describe the energy balances of each cyclone, consisting of the inflows: cold false air, solids from above, particle-laden gas from below and the effluent: total material flow at

the mixed temperature. The heat balance is also completed with the heat that was lost through the walls of the connector, barrel, and cone of the cyclone. Cyclone one is smaller than the others, it is also a twin setup so it has quadruple heat loss. The other cyclones $i \in \{2, 3, 4\}$, and even the separator share the same geometry, the whole tower is also a twin, hence all those heat losses are doubled.

$$0 = +Q_1^{\text{False Air}} + Q_{\text{Raw Meal}} + Q_2^{\text{After Riser}} - Q_1^{\text{s+se+g}} - 4UA_{\text{Small}} \cdot (T_1 - T_\infty) \quad (3.24)$$

$$0 = +Q_2^{\text{False Air}} + Q_1^{\text{After Pipe}} + Q_3^{\text{After Riser}} - Q_2^{\text{s+se+g}} - 2UA \cdot (T_2 - T_\infty) \quad (3.25)$$

$$0 = +Q_3^{\text{False Air}} + Q_2^{\text{After Pipe}} + Q_4^{\text{After Riser}} - Q_3^{\text{s+se+g}} - 2UA \cdot (T_3 - T_\infty) \quad (3.26)$$

$$0 = +Q_4^{\text{False Air}} + Q_3^{\text{After Pipe}} + Q_{\text{Separator}}^{\text{After Riser}} - Q_4^{\text{s+se+g}} - 2UA \cdot (T_4 - T_\infty) \quad (3.27)$$

Given that both phases travel through the connector, barrel, cone of each cyclone, these three parts may be considered lumped together, according to Eq.3.28. It is assumed that their mixed temperatures T_i approximate their interior bulk temperature field.

$$UA = UA_{\text{Barrel}} + UA_{\text{Cone}} + UA_{\text{Connector}} \quad (3.28)$$

Whereas the risers and pipes, equations 3.29-3.31, are instead spacially segregated. Wherein the interior bulk cools down along the axis, a phenomenon that can be modelled as an algebraic equation, by assuming that the temperature falls off *quite linearly*. Thus the arithmetic mean of the entry and the exit temperatures would be perfectly representative of the true distribution. Circumventing the need for simulating $1+3+3+1=8$ one-dimensional pipe-flow systems, in section 3.3.2, in every iteration of `fsolve`.

$$0 = +Q_1^{\text{s}} - Q_1^{\text{After Pipe}} - 4UA_{\text{Small}}^{\text{Pipe}} \cdot \left(\frac{T_1 + T_1^{\text{After Pipe}}}{2} - T_\infty \right) \quad (3.29)$$

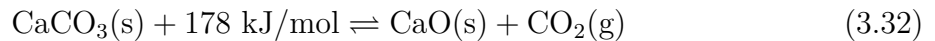
$$0 = +Q_i^{\text{s}} - Q_i^{\text{After Pipe}} - 2UA^{\text{Pipe}} \cdot \left(\frac{T_i + T_i^{\text{After Pipe}}}{2} - T_\infty \right) \quad i \in \{2, 3, 4\} \quad (3.30)$$

$$0 = +Q_i^{\text{se+g}} - Q_i^{\text{After Riser}} - 2UA^{\text{Riser}} \cdot \left(\frac{T_i + T_i^{\text{After Riser}}}{2} - T_\infty \right) \quad i \in \{2, 3, 4\} \quad (3.31)$$

This assumption of linear temperature fall-off is justified by the shortness of the pipes and risers, the slight cooling they undergo, and the naturally temperature-independent mechanism of conduction being the dominant thermal resistance comprising UA .

3.3.1.2 CALCINER

The calciner is considered a perfectly-mixed tank reactor that relies on the large surface area of finely ground raw meal combined with a turbulent gas flow to facilitate mass transfer of carbon dioxide out of the particles, in the presence of an open flame to facilitate heat transfer into the particles to feed the highly endothermic calcination reaction shown in Eq.3.32.



The calciner heat balance is similar to cyclone heat balance save for the reaction powers $+Q_{\text{Flame}} - Q_{\text{Calcination}}$. The thermal power of the flame as well as all of the combustion species was provided by a classified company report.

$$0 = +Q_{\text{Tertiary Air}}^{\text{INCOMING AIR \& SOLIDS}} + Q_4^{\text{After Pipe}} - Q_{\text{Calciner}}^{\text{OUTGOING}} + Q_{\text{Flame}}^{\text{REACTIONS}} - Q_{\text{Calcination}} - 2U A_{\text{Calciner}}^{\text{HEAT LOSS}} \cdot (T_{\text{Calciner}} - T_{\infty}) \quad (3.33)$$

$$0 = +Q_{\text{Calciner}}^{\text{s+g}} - Q_{\text{Calciner}}^{\text{After Duct}} - U A_{\text{Calciner}}^{\text{Duct}} \cdot \left(\frac{T_{\text{Calciner}} + T_{\text{Calciner}}^{\text{After Duct}}}{2} - T_{\infty} \right) \quad (3.34)$$

Since tertiary air is intentionally supplied to the calciner there is no explicit mention of unintentional false air. The calciner duct is very large and has highly articulated geometry, which would take a great deal of work to set up a heat-loss function for. So, it was expedited by simply taking the composite coefficient of heat transfer U for the barrel part of the standard-sized cyclone, and scaled it with the outer area of the whole calciner $>1700 \text{ m}^2$, provided by the company. Refractory thickness is unknown and the most important factor in heat loss.

3.3.1.3 SEPARATOR

The heat balances of the separator is a continuation of the preheater heat balances. All of the heat balances in the lumped system are solved simultaneously. Except for the separator pipe, since it is the input for the rotary kiln, which isn't formulated as algebraic equation and therefore can not be appended to the system of fifteen equations

$$0 = +Q_{\text{Separator+Kiln Hood}}^{\text{False Air}} + Q_{\text{Calciner}}^{\text{After Duct}} + Q_{\text{Kiln Gas}} - Q_{\text{Separator}}^{\text{s+se+g}} - 2U A \cdot (T_{\text{Separator}} - T_{\infty}) \quad (3.35)$$

$$0 = +Q_{\text{Separator}}^{\text{s}} - Q_{\text{Separator}}^{\text{After Pipe}} - 2U A_{\text{Pipe}} \cdot \left(\frac{T_{\text{Separator}} + T_{\text{Separator}}^{\text{After Pipe}}}{2} - T_{\infty} \right) \quad (3.36)$$

$$0 = +Q_{\text{Separator}}^{\text{se+g}} - Q_{\text{Separator}}^{\text{After Riser}} - 2U A_{\text{Riser}} \cdot \left(\frac{T_{\text{Separator}} + T_{\text{Separator}}^{\text{After Riser}}}{2} - T_{\infty} \right) \quad (3.37)$$

The separator is named and regarded as its own process unit for the convenience of the code, because the solids encounter the calciner between the separator and preheater. While in all other contexts, the preheater tower is consists of all cyclone separators, and sometimes the calciner as well.

3.3.2 ONE-DIMENSIONAL PIPE-FLOW SYSTEMS

The rotary kiln is the largest piece of equipment on the plant, the most energy intensive, and the most physically complex. But in this endeavour, it will suffice to regard it as a 1D pipe-flow BVP with a phasic counter-current heat balance. But before that can be modelled it is advantageous to explain a simpler version of the same problem. Which is that of the pipe that carries tertiary air from the cooler to the calciner.

Note that the gas travels from left to right, opposite to the direction depicted in the diagrams 1.1, 3.3, and 3.8.

3.3.2.1 TERTIARY-AIR PIPELINE

The heat balance over a long pipeline can be expressed as a boundary-value problem (BVP) composed of equations 3.38, and 3.39. It can predict the temperature of the effluent air $T_{\text{Tertiary Air}} = T(z = L)$ by breaking the pipe down into a finite set of points along its

length and then balances heat leaving and entering each of these axial slices (or points) of the pipe. And numerically solved using orthogonal collocation by MATLAB's **bvp4c** solver.

The differential equation 3.38 contains the following terms. The **conductive** term works to smooth out large gradients over short distances, it scales with the square of the pipe diameter. The **convective** term works to transport the hot air through the pipe. The **sink** term is a simplification of the three-dimensionality of the problem, the temperature of the fluid in a given slice is lumped (meaning no radial temperature distribution). The composite heat-transfer area UA_{Pipeline} governing the rate of cooling is obtained from the methods presented in section 2.3: Inner wall: Forced convection in turbulent pipe flow, conduction through cylindrical shells, forced external convection across horizontal cylinders. The division by pipe length L is necessary for the simplification to be valid, since each term must be in watts per meter.

$$\boxed{\underbrace{\dot{m}^{\text{Tertiary Air}} c_p^{\text{Air}}(T)}_{\text{Axial Convection}} \frac{\partial T}{\partial z} = \underbrace{k_{\text{Air}}(T) \frac{\pi D_i^2}{4}}_{\text{Axial Conduction}} \frac{\partial^2 T}{\partial z^2} - \underbrace{UA_{\text{Pipeline}} \frac{T - T_\infty}{L}}_{\text{Heat Sink}}} \quad (3.38)$$

$$\underbrace{T(z=0)}_{\text{Inlet}} = T_{\text{Secondary Air}} \quad \underbrace{\frac{\partial T}{\partial z}(z=L)}_{\text{Insulated at outlet}} = 0 \quad (3.39)$$

Semantically, the tertiary-air flow has cooled down to $T_{\text{Tertiary Air}}$ at the end of the pipeline. Before entering the calciner. The calciner is also fed additional false air. It is not known where along the pipeline the false air enters. So it is assumed that all false air enters the calciner itself, so that the pipeline only shows one cooling effect. It is preferable to have the model underpredict temperature.

3.3.2.2 ROTARY KILN

This unit is the most physically complex unit, for five reasons:

1. Dominant radiation in complex geometry
2. Rotation of the wall - causing alternating contact between the phases
3. Counter-current phasic flow
4. Chemical reactions
5. Significant heat loss

We cannot faithfully simulate the kiln in all its glory, along with the complete process. It is beyond the scope of this master thesis. However, it is possible to formulate a model that is capable of computing $T_{\text{Kiln Gas}}$ from $T_{\text{Calcined Meal}}$ and $T_{\text{Secondary Air}}$ (and mass balance solutions), by applying the following assumptions.

1. Using one-dimensional pipe-flow physics
2. Only simulating the gas-phase heat balance
3. Estimating the heat loss from gas bulk to outside air with composite heat transfer
4. Locking the bed's outlet temperature
5. Using the known heat of reaction as a sink term for the gas-phase heat balance
6. Treating the combustion reactions as a source term as a function of axial coordinate

The same general setup as for the tertiary-air pipeline may be used (Eq. 3.38 turns into Eq.3.40), with boundary conditions Eqs.3.41-3.42.

$$\boxed{\begin{array}{c} \dot{m}(z)c_p^{\text{Flue Gas}}(T)\frac{\partial T}{\partial z} = k(T)A_g\frac{\partial^2 T}{\partial z^2} - UA(T)\frac{T - T_\infty}{L} + q_{\text{Flame}}(z) - q_{\text{Calcination}}(z) - q_{\text{Bed}}(z) \\ \text{Axial Convection} \qquad \qquad \text{Axial Conduction} \qquad \qquad \text{Radial Heat Loss} \end{array}} \quad (3.40)$$

Where A_g is the cross-sectional area that the gas flows through. The rotary kiln is assumed to be filled by solids to 13% of the inner cross-sectional area $\pi D_i/4$. Where the kiln's inlet temperature is the solution to the mixed heat balance Eq.3.41. If plasma is used, then the heating will be concentrated in such a small domain that it is more accurate and convenient to add a fraction η_{Plasma} of the supplied power to the inlet, and while the rest of the plasma power is supplied along the kiln according to Eq.3.44. The physical description for this is that plasma converts electric energy into thermal energy through ionisation where the gas experiences an extremely high temperature (about 3000 °C) which gives way to endothermic dissociation reactions that store part of that thermal energy in chemical energy. As the gas cools along the kiln, the equilibrium shifts back, causing the ions to recombine and progressively release that enthalpy as heat, modelled as a source term.

$$0 = Q_{\text{Primary Air}} + Q_{\text{Secondary Air}} + Q_{\text{False Air}}^{\text{Kiln Hood}} + \underset{\eta_{\text{Plasma}}=0 \text{ for all tests}}{\eta_{\text{Plasma}} Q_{\text{Plasma}}^{\text{Kiln}}} - Q_{\text{Kiln Inlet}} \quad (3.41)$$

$$\begin{array}{cc} T(z=0) = T_{\text{Kiln Inlet}} & \frac{\partial T}{\partial z}(z=L) = 0 \\ \text{Inlet} & \text{Insulated at outlet} \end{array} \quad (3.42)$$

Since simulating the coupled, phasic heat balances is beyond the scope of this project, the heat fluxes $q_{\text{Flame or Plasma}}(z)$, $q_{\text{Calcination}}(z)$, and $q_{\text{Bed}}(z)$, in functions 3.43-3.46, will represent the phenomena, but decoupled from the temperature field $T(z)$ of the gas.

$$q_{\text{Flame}}(z) = Q_{\text{Flame}}^{\text{Kiln}} \times f_n(L_k - z, o) \quad (3.43)$$

$$q_{\text{Plasma}}(z) = (1 - \eta_{\text{Plasma}}) Q_{\text{Plasma}}^{\text{Kiln}} \times f_n(L_k - z, o) \quad (3.44)$$

$$q_{\text{Calcination}}(z) = Q_{\text{Calcination}}^{\text{Kiln}} \times f_n(z, o) \quad (3.45)$$

$$q_{\text{Bed}} = Q_{\text{Bed}} \sqrt{f_n(L_k - z, o)} \quad (3.46)$$

Where $Q_{\text{Flame}}^{\text{Kiln}}$ and temperature-enthalpy data of the bed material along the bed H_{Bed} is provided by HEIDELBERG reports, $Q_{\text{Calcination}}^{\text{Final}} = \frac{\dot{m}_{\text{CaCO}_3}^{\text{Separator, se}}}{M_{\text{CaCO}_3}} \Delta H_{\text{Calcination}}$, and $Q_{\text{Bed}} = \dot{m}_{\text{Separator}}^s \cdot (H_{\text{sk}}(T_{\text{Separator}}^{\text{After Pipe}}) - H_{\text{sk}}(T_{\text{Clinker}}))$ in a way that is both physically plausible and mathematically solvable.

$$f(z, o) = \begin{cases} \left(1 - \frac{z}{L_k}\right) \left(\frac{z}{L_k}\right)^o & f(z = L_k) = 0 \\ \left(1 - \frac{o}{o+1} \cdot \frac{z}{L_k}\right) \left(\frac{z}{L_k}\right)^o & \frac{\partial f}{\partial z}(z = L_k) = 0 \end{cases} \xrightarrow{\text{Normalise}} f_n(z, o) = \frac{f(z, o)}{\int_0^{L_k} f(\zeta, o) d\zeta} \quad (3.47)$$

The distributions are such that one end must have non-zero value or non-zero gradient. Flame was chosen to be the only one with a non-zero gradient. But this is a completely arbitrary choice.

Shown in Fig.3.9 is the way that the normalized distribution $f_n(z, o)$ is used to represent the relative heat fluxes along z , for flame and for calcination, individually. The gas

enters from the left where it is inflamed until reaching halfway across. The partially calcined meal enters from the right and the calcination reaction finalizes as the cold bed is met by the counter-current flue-gas stream. Which works to sharply cool down said gas due to endothermism, and works to feed it extra CO_2 mass flow.

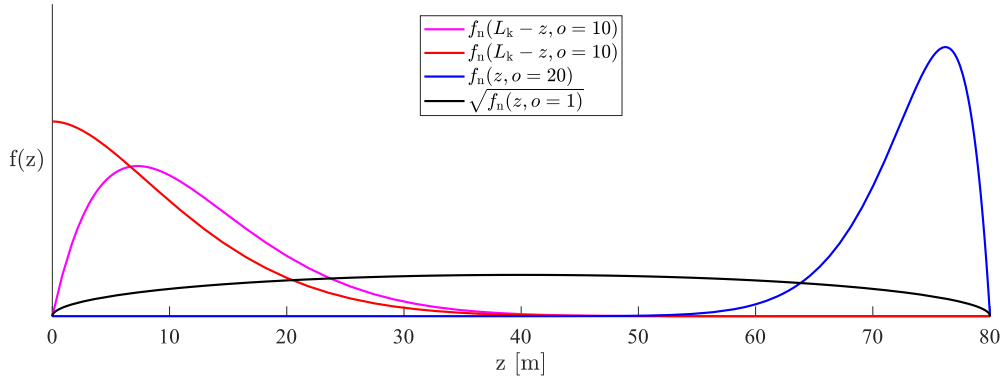


Figure 3.9: The *magenta* line is the plasma dissociation heat-flux source, the *red* line the flame heat-flux source, *blue* line is the calcination heat-flux sink, and the *black* line is to show the cumulative gas flow that is added through volatilisation of solid fuels (by combustion) and CaCO_3 (by calcination). Note that the graphs only indicate the individual relative distributions along z .

Another benefit of having the distribution respond to the parameter o , in that a greater order o makes f_n pointier, is that the plasma torch is characteristically shorter in length with a greater peak gas temperature - to the detriment of thermal efficiency. In short, the model may capture the effects of a fuel switch.

Reducing the order of differential equations is possible to do if the Péclet number 3.48 is large. Meaning the convection and length of the system overpowers the conductive mechanism. Then the conductive term may be cancelled with callous disregard. Sparing you from solving a BVP. Then the 1D pipe-flow system may be solved using MATLAB's differential-equation solver `ode89`.

$$\text{Pe}_L = \frac{G \times c_p \times L}{k} \quad (3.48)$$

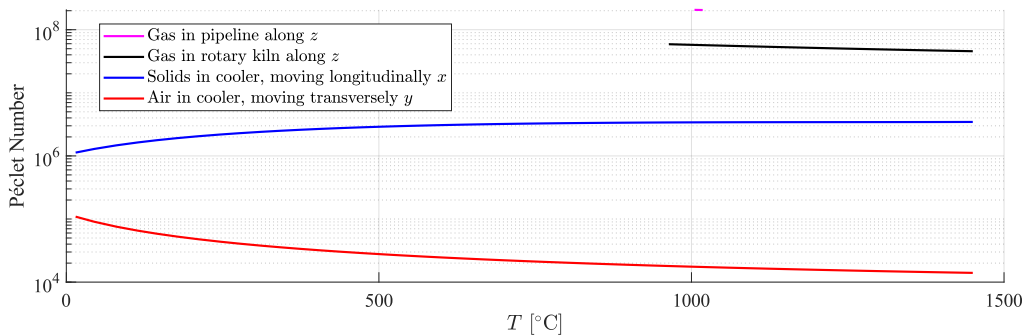


Figure 3.10: Showing Péclet numbers for all differential equation in the process. The observed values are always much larger than unity. Leading to the negligible contribution of axial conduction.

3.3.3 COOLER

The cooler unit operation consist of a conveyor belt, an array of fans, and two headers. Hot clinker is cooled rapidly by a stream of cold air from below. The cross-flow configuration is modelled as a fixed bed with convective-conductive partial differential equations for each phase with a heat-exchange source term. It was pragmatic to neglect longitudinal conduction $\frac{\partial^2 T}{\partial x^2} \approx 0$ as this allows the efficient, built-in solver named `pdepe`, to be used. Which solves a transient 1-D PDE. But the model loses an effect of mixing and exergy destruction that is present in the real world. However, the calculated Péclet number of the solids along x is much larger than unity for the base case, shown in Fig.3.10.

$$G_s c_p^s \alpha_s \frac{\partial T_s}{\partial x} = \frac{\partial}{\partial y} \left(k_s \alpha_s \frac{\partial T_s}{\partial y} \right) - h \frac{T_s - T_a}{X} \quad (3.49)$$

$$0 = \frac{\partial}{\partial y} \left(k_a \alpha_a \frac{\partial T_a}{\partial y} - G_a c_p^a \alpha_a T_a \right) + h \frac{T_s - T_a}{X} \quad (3.50)$$

With the following boundary conditions:

$$T_s(x = -L_1, y) = T_{\text{Clinker}} \quad \frac{\partial T_s}{\partial y}(x, y = 0) = 0 \quad \alpha_s k_s \frac{\partial T_s}{\partial y}(x, y = H) = U A_{\text{Roof}} \frac{T_s(x, y = H) - T_\infty}{L} \quad (3.51)$$

$$T_a(x = -L_1, y) = T_{\text{Clinker}} \quad \frac{\partial T_a}{\partial y}(x, y = 0) = 0 \quad \frac{\partial T_a}{\partial y}(x, y = H) = 0 \quad (3.52)$$

Where the heat-transfer area $U A_{\text{Roof}}$ is obtained from the composite heat transfer using pure radiation from solids surface to ceiling, conduction through plate, and natural convection on horizontal plate and radiation. Where $\alpha_s \approx 50\%$ is the volume solids in relation to total volume and its complement is of gas. The fixed-bed assumption works when the weight of solids far exceeds the drag forces that try to lift the particles. Then the maximal packing fraction is known for a monodisperse suspension of a given sphericity. If the converse was instead true, the whole master thesis would be entirely consumed by fluidized-bed modelling in CFD.

The phases will move perpendicularly, the most useful movement parameter is the superficial mass velocity G [kg/m²s] ($G = \rho v$), presented in Eq.3.53. Mass flow rates are already known at this point and they must be upheld in the energy balances. Those must be divided by the average amount of area that each phase can permeate through along its respective flow-wise direction. This can be argued from the geometry of the box with length L , width W , and height H , and a preset, solid volume fraction α_s , and since air is the only other phase in the system $\alpha_a := 1 - \alpha_s$. Solid volume fraction is assumed to be constant within the cooler. The average permeation area is the volume of the phase in question divided by the length for the solids and height H for air.

$$G_a = \frac{\dot{m}_a}{LW\alpha_a} \quad G_s = \frac{\dot{m}_s}{HW\alpha_s} \quad (3.53)$$

The phasic heat-exchange coefficient h describes the amount of heat that exchanged between the air and the solids locally in each cell of the mesh. Its formula (Eqs.3.55) was taken [12], and its notation for the characteristic length X Eqs. 3.54 (not to be confused with conversion).

$$X := \frac{\text{Box Volume}}{\text{Interface Area}} = \frac{1.5^{1/3} \langle d_p \rangle}{6\alpha_s} \quad \text{Re}_X = \frac{G_a X}{\mu_a} \quad (3.54)$$

$$\text{Nu}_X = 8.74 + 9.34 (6\alpha_s \text{Re}_X)^2 \text{Pr}_a^{1/3} \quad h = \frac{k_a}{X} \text{Nu}_X \quad (3.55)$$

The outlet temperatures can be calculated as line integrals (Eqs. 3.56-3.58) – since the width, mass velocities and volume fractions are uniform in the domain. Additionally, the cooler area efficiency η_g can be calculated (Eq.3.59).

$$T_{\text{Cold Clinker}} = \frac{1}{H} \int_{0\text{m}}^H T_s(x = L_{\text{Vent}}, y) dy \quad (3.56)$$

$$T_{\text{Secondary Air}} = \frac{1}{L - L_{\text{Vent}}} \int_{L_{\text{Vent}}-L}^{0\text{m}} T_g(x, y = H) dy \quad (3.57)$$

$$T_{\text{Vent Air}} = \frac{1}{L_{\text{Vent}}} \int_{0\text{m}}^{L_{\text{Vent}}} T_g(x, y = H) dy \quad (3.58)$$

$$\eta_g = \frac{T_{\text{Secondary Air}} - T_{\infty}}{T_{\text{Hot Clinker}} - T_{\infty}} \quad (3.59)$$

3.3.3.1 EMERGENCE OF COMPOSITE HEAT LOSS

Recall the equations describing convective heat transfer. There were isobaric, specific heat capacity c_p , thermal conductivity k , dynamic viscosity μ , and Prandtl number Pr . All of these must be evaluated at the temperature of the film at the given location. Film temperature is the arithmetic mean of the bulk and surface temperatures $T_{\text{fi}} = \frac{T + T_{\text{wi}}}{2}$ (inner film), $T_{\text{fo}} = \frac{T_{\text{wo}} + T_{\infty}}{2}$ (outer film).

The mechanisms work in series (so thermal resistances are summed Eq.3.60) over each part Eq.3.63, and the parts work in parallel (energy balances of section3.3). Where 'parts' include:

Lumped Parts	Linear-Temperature-Profile Parts	Differential-Temperature-Profile Parts
Barrels	Risers	Pipeline (for tertiary air)
Cones	Pipes	Kiln
Connectors		Cooler Roof

$$R_{\text{Total}}^{\text{Part}}(T_{\text{wi}}, T_{\text{wo}}) = R_{\text{Inner}}^{\text{Part}}(T_{\text{wi}}) + R_{\text{Wall}}^{\text{Part}} + R_{\text{Outer}}^{\text{Part}}(T_{\text{wo}}) \quad (3.60)$$

$$\frac{T - T_{\text{wi}}}{R_{\text{Inner}}(T_{\text{wi}})} = \frac{T - T_{\infty}}{R_{\text{Total}}(T_{\text{wi}}, T_{\text{wo}})} = \frac{T_{\text{wo}} - T_{\infty}}{R_{\text{Outer}}(T_{\text{wo}})} \quad (3.61)$$

$$[T_{\text{wi}}, T_{\text{wo}}] = \text{fsolve}(@\text{Eq.3.61}, T_{\text{Guesses}}, \text{options}, T) \quad (3.62)$$

$$UA_{\text{Part}}(T) = \frac{1}{R_{\text{Total}}(T_{\text{wi}}(T), T_{\text{wo}}(T))} \quad (3.63)$$

But solving non-linear algebraic equations during each iteration, merely to access information on film temperatures is a waste of computational time. So, the strategy is to

1. Feed material-property data directly into the expressions for thermal resistances
2. Fit polynomial functions to the calculated resistances (1) with reasonable temperature ranges that correspond to inner and outer wall temperatures
3. Build the composite-wall heat balance (system of non-linear algebraic equations Eqs.3.60&3.61) using the polynomials R (2)
4. Define a linearly spaced vector of internal-bulk-temperature (T) values, in the global range (2), with about ten elements
5. Loop over the temperature vector T (4) and obtain the corresponding wall temperatures by numerically solving the composite-wall heat balance (3) Eq.3.62
6. Evaluate the polynomial functions describing thermal resistances (2) at their corresponding wall temperatures (5)
7. Add all resistances (6) together, into one vector of total resistance, invert it to give the vector for composite heat-transfer area UA
8. Fit a new polynomial for UA (7) to the internal-bulk-temperature vector T (4), rendering Eq.3.63
9. Plot the result to inspect goodness of fit of (8) to (7) (see Fig.3.11)

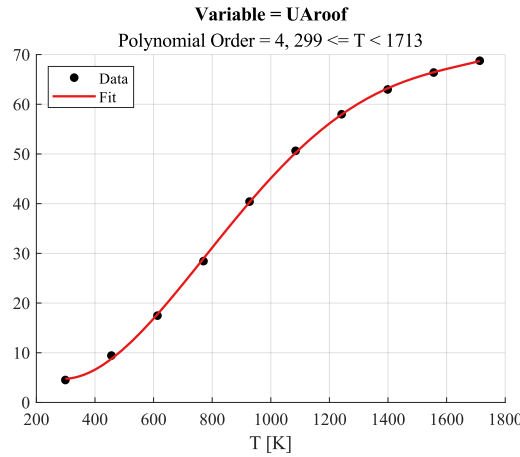


Figure 3.11: Result of the method. This example is the composite heat-transfer area UA for the roof of the cooler. The polynomial captures the T^4 -ramp-up - indicative of radiation, and the subsequent fall-off - which is telling for an increasingly dominant conductive resistance.

4 RESULTS

Presented are results of some important variables from solving all of the mass and energy balances. The base case is as follows:

- 75% CaCO_3 purity in the 383-ton/hr, 60- °C raw-meal feed
- Dry, 14.85-°C ambient air
- 0.04 as universal discharge coefficient controlling false-air ingress
- $\eta_i = 80\%$ for all but the top-most cyclones ($i = 1$) which is assumed to have half the mass loss ($\eta_1 = 90\%$ by default)
- Primary, secondary, tertiary, and vent air flows are 0.04, 0.63, 0.34, and 0.05 respectively in normal cubic meters of air per kg of clinker, but Heidelberg’s 2022 report says that an unknown amount of false air enters the calciner to supply enough oxygen, air factor was set to 1.15.
- CCFR=0.9, calcination reaction consumes 90% of the power that is provided by the calciner flame
- Effective clinker particle diameter is set to be 3 cm in the cooler. It is most important parameter determining the cooler efficiency $\eta_g = 60\text{-}70\%$

4.1 RESULTS OF MASS BALANCES

The most important solid streams are the inputs ash and raw meal, the outputs lost meal and clinker, and the calcined meal which connects the tower to the kiln. Shown in table 4.1. The solids mass balances were identical between flame and plasma. One might expect the ash to be unique to the flame process, but it is not. The Heidelberg engineer said that the compounds contained in ash play a role in clinker formation. So the plasma system is modelled as having ash injection as well.

Table 4.1: Evolution of the solids composition along the process.

	$\dot{m}$ [ton/h]	w [%]				
	Total	CaCO_3	CaO	SiO_2	Fe_2O_3	Al_2O_3
Ash	5	0	0	80	10	10
Raw Meal	383	75	0	15	7	3
Lost Meal	49	75	0	15	7	3
Calcined Meal	337	37	31	19	9	3
Clinker	229	0	61	24	11	4

The most important gas flows and compositions are shown in table 4.2. It is expected that the CO_2 concentration is much higher in the plasma process, however some papers assumed it was 100% CO_2 . But zero false air is not realistic for production scale. Given that there are many incoming air streams that differ between the two processes, thus a total mass flow of air was omitted.

Table 4.2: Mass flow and compositions of the gas mixture at the Exhaust stream shown for the flame process in Fig.3.3, which is equivalent to the cooling-gas stream in the plasma process Fig.3.8.

	$\dot{m}$ [ton/h]	w [%]						
	Total	N ₂	O ₂	Ar	CO ₂	H ₂ O	HCl	SO ₂
Air	-	75.51	23.14	1.28	0.06	0	0	0
Exhaust	449	66.58	3.39	0.9	23.85	5.11	0.03	0.15
Cooling Gas	387	11.97	3.67	0.2	84.16	0	0	0

4.2 RESULTS OF HEAT BALANCES

The solutions of the heat balances are presented as a bar graph showing effluent temperatures across all units, in Fig.4.1. The results have been simplified by omitting the temperatures of the solids coming out of the cyclone pipes and the particle-laden gas exiting the cyclone risers, since the temperature differences were small. However the temperature drop through the calciner duct was larger due to its high surface area >1000 m². Which is the reason for the high heat loss suffered by the calciner, heat losses shown in Fig.4.2. The differential units such as the kiln, "cooler1" (roof of the cooler that takes secondary and tertiary air), pipeline, cooler vent where calculated as is the integral of the heat-sink term of gas temperature fields along the full lengths.. In table 4.3 the results are compared against two independent and conflicting sources of information as to what the temperatures ought to be.

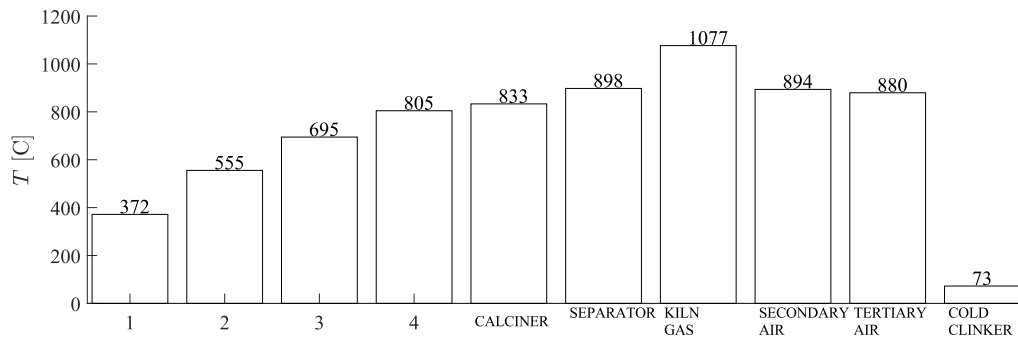


Figure 4.1: The numbers above the bars display the effluent temperatures of each unit identified by the index. The bars ease comparison between units, it shows how the temperature increases as the solids pass down through the preheater's four cyclone steps. Note that the values do not exactly match those of the base case, in later table entries, this is the regrettable fallout of minor tweaks and improvements of the code during the experimentation.

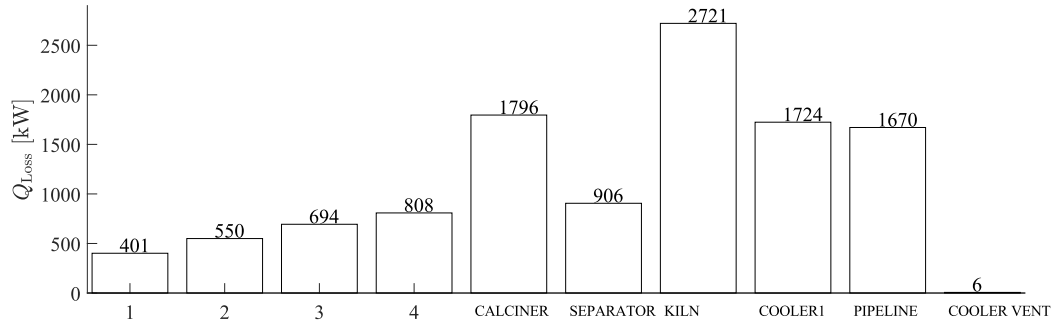


Figure 4.2: Heat losses of each unit in kilo watts. It is surprising how similar the heat losses are along the preheater, given that the top step has nearly double the surface area of the others. Although, it is expected that the kiln has the greatest heat loss of all.

Table 4.3: Temperatures [$^{\circ}\text{C}$] of outlet streams in the process. Units are ordered from left to right, generally according to the flow path the solid phase takes. The middle row is for the base case (same information as in Fig.4.1) but shown in table format to assist comparison with measurements and expectations.

	T [°C]									
	Preheater				Calciner	Sep.	Kiln Gas	Sec. Air	Ter. Air	Cold Clinker
General Fig.1.1	290	480	650	800	890	950	1150	1000	-	-
Base Case	375	557	691	795	820	887	1072	878	864	70
Gotland 2022	408	593	664	749	868	-	1080	900	887	172

4.3 SENSITIVITY ANALYSIS

This is done to probe the model for information about the importance of different physical phenomena and observing what effects they may have on the solution space.

4.3.1 FALSE-AIR EFFECT

The amount of false air that enters the system had a major effect on outlet temperatures. Firstly, the direct cooling effect, secondly the cumulative addition of gas-phase thermal inertia has the effect of transferring more heat to subsequent cyclones further up in the tower. Whereby, adding more false air causes the separator to drastically cool down, while also causing the top cyclones' temperature to increase. The latter effect can be observed in table 4.4. Wherein the top preheater cyclone (left-most row) heats up with increased discharge (ingress), while the bottom units instead cool down.

However, it was found that the base-case experiments stood on some shaky ground (discussed in 5.1.1). Rectifying the problem and investigating its impact yielded table 4.5. Where significantly larger (more realistic) discharge coefficients were tested to obtain a sensible mass fraction of O_2 in the exhaust stream, which was only recoded for this version of the code.

Table 4.4: The base-case run shown the middle, compared to no and to double false air. The last three columns do not and should not change because the hot-clinker temperature is locked.

C_d	T [°C]									
	Preheater				Calciner	Sep.	Kiln Gas	Sec. Air	Ter. Air	Cold Clinker
0	364	548	690	805	828	904	1063	878	864	70
-0.04	-11	-9	-1	+10	+8	+17	-9	0	0	0
0.04	375	557	691	795	820	887	1072	878	864	70
+0.04	+10	+7	-1	-10	-8	-16	+10	0	0	0
0.08	385	564	690	784	812	871	1082	878	864	70

Table 4.5: Swapping the position of the kiln hood along with its gauge pressure according to table3.4.

C_d	T [°C]								Exhaust	
	Preheater				Calciner	Sep.	Kiln Gas	Sec. Air	$\dot{m}_g$ [kg/s]	w_{O_2} [%]
0	356	535	675	788	816	887	1036	878	120	2.0
-0.30	0	+6	+14	+21	+16	+27	+29	0	-8	-1.4
0.30	356	529	661	768	801	860	1007	878	129	3.4
+0.30	-1	-7	-13	-19	-15	-25	-28	0	+8	1.2
0.60	355	522	648	749	786	835	979	878	137	4.6

4.3.2 RAW-MEAL-MASS-FLOW EFFECT

Raw-meal inflow is the most imbedded parameter in the code. Changing it affects nearly every aspect of the plant, apart from the cooler outlets as the hot clinker temperature has been hard-coded to always be 1450 °C and the air flows are set in accordance to the mass flow of clinker. Results are shown in table 4.6.

Table 4.6: Comparing the resulting temperatures between a reduction and an increase in raw-meal feed.

$\dot{m}$ [ton/hr]	T [°C]									
Raw Meal	Preheater				Calciner	Sep.	Kiln Gas	Sec. Air	Ter. Air	Cold Clinker
363	403 °C	597	738	846	852	941	1180	879	865	66
-20	28	41	47	51	32	54	108	2	1	-4
383	375	557	691	795	820	887	1072	878	864	70
+20	-24	-36	-42	-45	-29	-48	-94	-2	-1	3
403	351	521	649	750	792	839	978	876	863	73

4.3.3 PLASMA

The plasma-powered process will have less gas flow, and it will consist mostly of CO₂ with some recirculating false air as well. Table 4.7 compares the temperatures, wherein the prevailing sentiment is that plasma gives improved availability of heat in the reactors

and a greater difference in temperature between the cyclones, indicative of less gas heat capacity. The hottest units being even hotter will however incur greater process-wide heat losses shown in table 4.11.

Table 4.7: The difference between the power systems $\Delta = \text{Plasma} - \text{Flame}$.

	$T \text{ [}^\circ\text{C]}$									
	Preheater				Calciner	Sep.	Kiln Gas	Sec. Air	Ter. Air	Cold Clinker
Flame	375	557	691	795	820	887	1072	878	864	70
Δ	-35	-31	-10	+21	+80	+65	+54	+122	+120	-12
Plasma	340	525	680	816	900	953	1126	1000	984	58

4.3.4 SEPARATION-EFFICIENCY EFFECT

Separation efficiency is the fraction of solid mass that is collected by a cyclone in proportion to how much flows in. Higher efficiency (lower mass loss) makes the plant produce more clinker for the same raw meal. This is shown in the last column of table 4.8. The preheater's internal solid streams exceed the raw-meal feed (referring to the same table). This is expected for recirculation.

The stream temperatures in table 4.9 show that that increased recirculation leads to greater temperatures contained in the system, due to less raw meal finding its way to the heat sources. Where the constant power outputs of the calciner and kiln skew the results. The model could show other, less obvious, effects if it was programmed to scale the fuel deliveries to the mass flow of CaCO_3 in hot meal, and the mass flow of calcined meal. Another notable result is that neither result (tables 4.8-4.9) show a linear relationship with the mass-loss variable $1 - \eta$, it speaks to the emergent properties of the matrix equation 3.8.

Table 4.8: Solid mass flows in each unit in relation to the raw-meal inflow at 383 t/h or 106.39 kg/s. So, for instance, the solids mass flow from the kiln were $0.60 \times 383 = 229.8$ t/h, given 20% mass loss for all but the top preheater step, which always incurs half the loss, due it consisting of four parallel cyclones, rather than two.

$\frac{\text{Entrained}}{\text{Input}} \text{ [%]}$	$X \text{ [%]}$	$\dot{m}/\dot{m}_{\text{Raw Meal}}$					
Cyclones	Calciner	Preheater Outlets				Calcined Meal	Clinker
10	53	1.12	1.18	1.18	1.14	0.86	0.65
-10	-2	-0.17	-0.26	-0.24	-0.16	-0.02	0.05
20	54	1.29	1.44	1.42	1.31	0.88	0.60
+10	5	0.26	0.39	0.31	0.15	-0.02	-0.07
30	60	1.55	1.84	1.72	1.46	0.86	0.53

Table 4.9: Mass losses, conversions X of CaCO_3 in the Calciner, and Temperatures in $^\circ\text{C}$ for the units.

$\frac{\text{Entrained}}{\text{Input}}$ [%]	X [%]	T [$^\circ\text{C}$]						
Cyclones	Calciner	Preheater				Calciner	Sep.	Kiln Gas
10	53	343	518	645	741	792	822	922
-10	-2	-32	-39	-46	-53	-28	-65	-150
20	54	375	557	691	795	820	887	1072
+10	+5	+53	+62	+74	+88	+50	+110	+272
30	60	428	619	765	883	870	997	1344

4.3.5 CONVERSION EFFECT

The local conversion of CaCO_3 in the calciner is the user-specified parameter X . Heidelberg Materials typically aim for 90% conversion. But since this parameter is hands-down the most sensitive with respect to calciner and kiln-gas temperatures. The real conversion that a system attains is strongly coupled to the temperature and vice versa, coupling that would involve multiphase-CFD modelling (well beyond the scope of this project). Still, one can set up a linear heat balance using the most important constant, that being the calciner flame power $Q_{\text{Flame}}^{\text{C}}$. Assuming that power to be tailor-made to overcome the rate of endothermic calcination reaction $\dot{n}\Delta H_{\text{R}}$; a relationship between these two quantities was defined as Calciner Calcination-reaction-to-Flame power Ratio CCFR. Table 4.10 presents the resulting conversion and temperature when changing the CCFR by 0.2.

Table 4.10: Adjusting the- conversion X in the calciner. Higher conversion leads to a nearly linear decrease in temperature at the tower, but a linear increase at the kiln. This is expected. The cooler-outlet temperatures are unchanged from the base case.

CCFR	X [%]	T [$^\circ\text{C}$]						
Calciner		Preheater				Calciner	Sep.	Kiln Gas
0.7	41	365	541	671	772	894	860	840
-0.2	-13	-10	-16	-20	-23	+74	-27	-232
0.9	54	375	557	691	795	820	887	1072
+0.2	+14	+9	+14	+17	+21	-80	+24	+245
1.1	69	384	570	708	815	740	911	1317

If you were to force 90% conversion upon the calciner. Then an over-prediction of the available heat for calcination is made implicitly. Those unrealistic boundary conditions are, without any guardrails, passed on to the rotary kiln. Letting a numerically sensitive BVP run amok with very low cooling from remaining calcination, which causes it to pass unrealistically hot gases (1500°C) to the tower, heating it up the temperatures to offset the extreme cooling that occurred. Closing a positive feedback loop which may ultimately allow the calciner to look as though 90% conversion is achievable and that something else went wrong. But the instability was only experienced when including axial conduction (BVP rather than IVP) and for some configurations of the distributions $f(z, o)$ (under kiln method in 3.3.2.2).

Table 4.11: Heat losses in each unit in kW. The difference between the power systems $\Delta = \text{Plasma} - \text{Flame}$. The total heat losses suffered by the plant is still a fraction of the fire power, about 200 000 kW.

		$UA \cdot (T - T_\infty)$ [kW]									
	Total	Preheater				Calciner	Sep.	Kiln	Cooler Roof	Pipeline	Vent Roof
Flame	11203	405	551	690	798	1767	895	2766	1685	1640	6
Δ	+762	-40	-33	-11	+22	+178	+68	+461	-117	+234	-2
Plasma	11965	365	518	679	820	1945	963	3228	1568	1875	3

4.4 DIFFERENTIAL EQUATIONS

The temperature profiles (profile for base-case setup shown in Fig.4.3) that are routinely obtained from the developed model (section 3.3.2.2) are markedly higher than one might expect the gas-temperature maximum of a real kiln to be, which is around 2000 °C. However the outgoing-gas temperature is in accordance with measurements. Because of the largest energy consumer being the calcination of the remaining CaCO_3 in the calcined meal. The decoupling of the phases means that the temperature distribution is merely a way to estimate the total heat losses to the surroundings. Therefore, if you the reader has access to experimental data and/or a detailed heat-transfer model of the rotary kiln (on Gotland, working at the operating conditions of the base case) then compare this model's prediction of the kiln's heat losses to the surroundings (Fig.4.2), rather than the temperature distribution itself.

The solution of the coupled partial-differential equations of solids (clinker) and gas (air) phases is presented as a 2D contour (Fig.4.5). Representing cross-sectional slices of the porous bed. Where the solids are moved slowly to the right along a conveyor belt. Whereas the gas is blown upwards through the bed, perpendicularly.

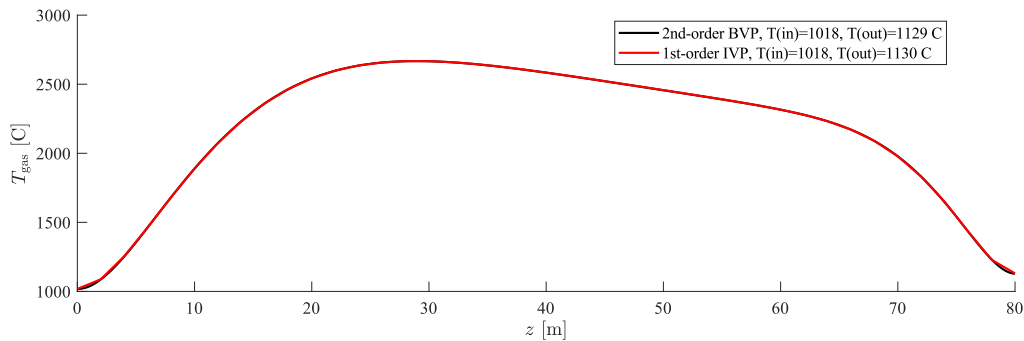


Figure 4.3: Rotary-Kiln, bulk-gas axial temperature profile. It is also shown that the kiln model can be solved as a Boundary Value Problem, but also as a 1st-order IVP without axial conduction, as described in 3.3.2.2.

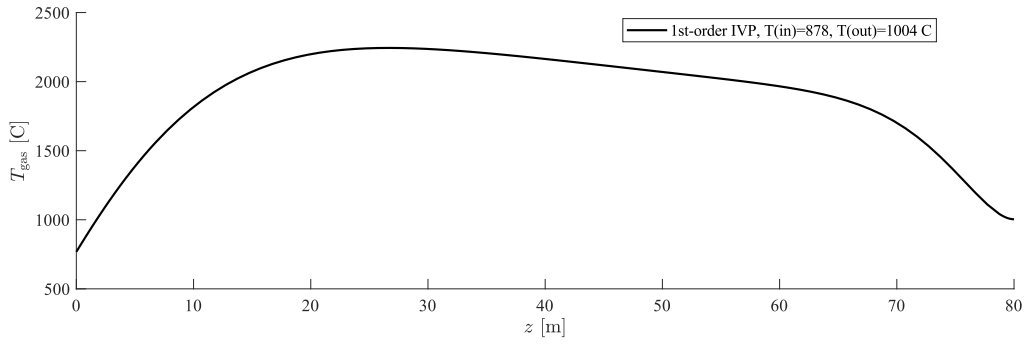


Figure 4.4: Kiln bulk-gas axial temperature profile. For a setup using flame, and a different setup overall. Beware, the legend displays the temperatures of secondary air and kiln gas but asserts that the former is $T(\text{in})=878^\circ\text{C}$ which is not technically true. The graph indicates the correct inlet temperature around $700\text{--}800^\circ\text{C}$.

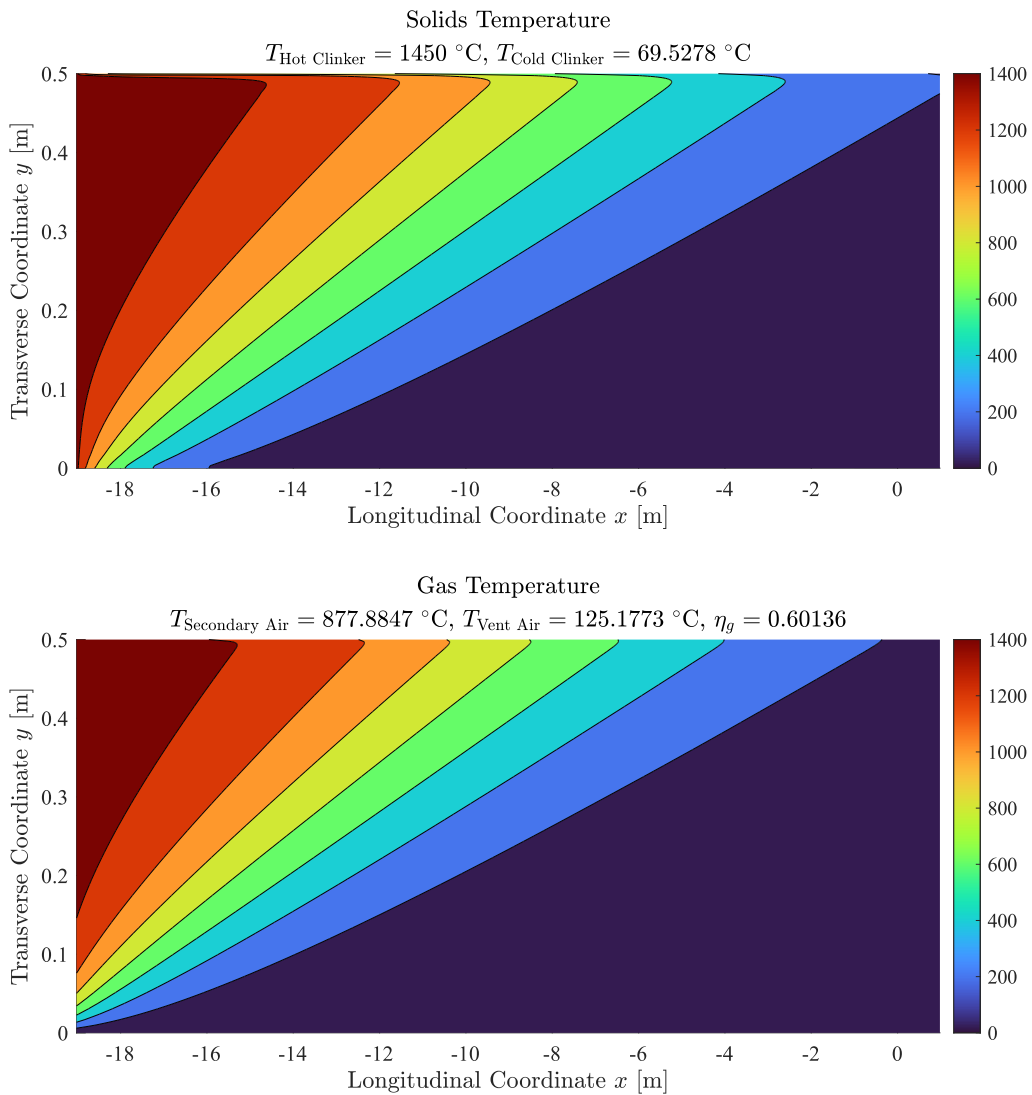


Figure 4.5: The phasic temperature contours in the cooler, the colours correspond to the same absolute temperatures. The outlet temperatures are shown in the titles where both $\dot{m}_{\text{Secondary Air}}$ and $\dot{m}_{\text{Tertiary Air}}$ exit the cooler at $T_{\text{Secondary Air}}$, on the boundary $x \leq 0$, $y = H$.

5 DISCUSSION

The mass-energy balances over the core components of the contemporary cement process were modelled and solved. The model is capable of predicting the stream temperatures across the plant to a reasonable level, given the uncertainties in the measurements. The model does not appear to lack any crucial phenomena. While, of course, it is impossible to prove a negative. There are a finite set of important physical phenomena (heat losses, temperature-dependant material properties, conduction, convection, radiation, mixing, separation, reactions, etc.). And the model contains considerations for the phenomena that range from rudimentary estimations of provably small effects, to the first-principles thinking that is underlying mass and energy balances.

The resulting codebase is hierarchical in the sense that phenomena are expressed as functions, and functions call upon other, more foundational functions, saving repeated lines. While similar units are combined into one system with a shared solution strategy.

5.1 SOURCES OF ERROR

Information about wall thicknesses and refractory conductivity in all but the rotary kiln was devastatingly scarce. But the model turned out to have predictive power nonetheless. This is most likely the cause of good insulation that render the effects of heat losses small.

False-Air calculations were derived from Bernoulli's equation and continuity, but were propped up by gauge-pressure measurements P_i (table 3.4) that have uncertainties and are assumed to remain constant across all tests. False-Air ingress was then also controlled with a physics-backed coefficient of discharge which was manually set, such that a reasonable amount of false air would enter the system.

The assumption of dry air may be challenged as the plant is situated next to the ocean, and informal tests showed that it had non-zero impact on temperatures. Most likely wrought by the mechanistic approach toward calculating false air.

5.1.1 KILN-HOOD LOCATION

The hood was erroneously thought to be at the cold end of the kiln (next to the tower). But this configuration leads to a $>2 \text{ m}^2$ area sucking in air with >1000 pascals of gauge pressure in the centre of the system, so the entire plant becomes very cold and full of air if the discharge coefficient is even moderately large. Thus, it had to be set very low to predict other effects. It is regrettable that the mistake was found after obtaining all results. However, this does not invalidate the model nor the results, as swapping a false-air source and increasing C_d to give the same overall air ingress, did not make enough of a difference to change the overall narrative.

5.1.2 CONVERSION

The calciner is really nothing more than big duct where fuel is burned, treating it as a continuously-stirred tank reactor did not turn out amazingly well. It would be possible to set a calciner conversion and a separator conversion. It would mean that the separator's

heat balance also contains calcination cooling. Then, the partially-calcined meal would get a second blast of heat from the rising kiln gas. Allowing more conversion to occur without cooling the calciner stream to temperatures below what is chemically possible. This would allow more conversion (current result is 50%, while measurements indicate 90%), without cooling the calciner, and shifting the burden of calcination from the rotary kiln to the separator. It would make the kiln gas hotter as well, (1050 °C now, measurements say 1150 °C). Informal testing suggest that calciner and separator temperatures were around 900 °C, but the kiln gas ended up being 1500 °C. Which suggests that the informal test failed to balance the heat properly.

5.2 PLASMA RETROFIT

The existing plants may be retrofitted with plasma torches and an alternative setup to take advantage of the low gas flow rates that are otherwise required for oxygen. Such a retrofit would confer greater energy efficiency, but the kiln walls in particular may struggle to withstand the elevated temperatures and temperature gradients, due to plasma. For whomever decides to undertake the challenge, they may experience difficulties with the calciner, as the backwards calcination reaction is favoured in the high partial pressure of CO₂.

5.3 NEXT-GENERATION CEMENT PLANT

The first step towards designing a plasma-powered cement plant, from scratch, should likely concern the choice of clinker cooler. The grate cooler is a dated device that destroys a great deal of exergy by design, due to its cross-flow configuration and its addiction to large quantities of cold air. The future system may reuse the waste heat in from the clinker to preheat raw meal, in lieu of secondary and tertiary air. Using a different kind of heat exchanger that works by transferring heat from one granulate to another granulate directly through radiation or through wall conduction, without an exergy-destroying gas.

6 CONCLUSIONS

The cyclones' separation efficiency affects the clinker output. Lost raw meal out of the top cyclones is not an insignificant mass loss. While the separators entrainment rate increases the unintended recirculation, which will inherently increase the conversion as the local mass flow of solids passing through the calciner increases.

The heat losses will generally scale linearly with temperature due to the liberal use of thick refractories in the construction. Leading to conductive resistance dominating. Especially for the hotter units, given that they are designed to insulate the best, and have vanishingly small radiative and convective resistances against the inner and outer surfaces.

The plasma system had more available heat by being alleviated from extra gas flow, as required for combustion. The experiments to compare the two power mechanisms were run with identical setups. The air flow only differed in false air to the calciner, flame system needed 9.5 kg/s while plasma needed none. But the base setup seemed to have overly large secondary air flow 0.63 Nm³/s per kg/s clinker. The plasma system would be served better by less secondary air, no primary air, and more vent air to compensate for the cooling deficit. With or without those changes the plasma system still manages to have higher temperature in the reactors, which would likely facilitate calcination in an otherwise unacceptably high concentration of CO₂.

Emergent behaviour was generally spotted in the cyclones, because of their strong coupling with each other. One example of emergence is the temperature at the top of the preheater, which became hotter when double false air was let in to each unit. Contrary to the expectation that cold air everywhere would cool everywhere more. All paragraphs under conclusions may arguably be attributed to emergent behaviour since none of these effects would be observable if models were developed and tested in isolation.

6.1 FUTURE MODELLING WORK

The main deficiencies of the current model are: false air; momentum transfer; some unconfirmed sizes of calciner, pipeline, and cooler; lack of model for separation efficiencies; the rotary kiln; Calciner.

6.1.1 ROTARY-KILN UPGRADES

Implementing coupled gas-bed heat balances, necessitates a great deal of heat transfer mechanisms: convection and radiation from gas to bed, gas to wall, conduction and radiation from wall to bed, there are transient, three-dimensional effects, rotation, bed circulation, clinker reactions coupled to emissivities, viscosity, conductivity, particle size distributions, bed speed, et cetera.

6.1.2 CALCINATION KINETICS

One may adapt the model to account for the kinetics and delocalise the reaction from the unit, having a second conversion factor for the separator and perhaps even the preheater. This idea was brought up at an early stage of development, but was shot down because

it seemed prohibitively difficult to accomplish. However, model now works by solving the balances in a decoupled and sequential way, which paves the way for an expansion of this scope.

REJECTION OF ARTIFICIAL INTELLIGENCE

I declare that not a single word, equation, table nor figure in this document was generated by any large language model. Nor was any such tool used during the process of programming, modelling, conceptualising, writing, reading, re-writing, nor re-reading. The reason for my hardline stance is that I fear losing my ability to think critically, by taking the path of least resistance and succumbing to the certainty of the current chatbots. Although, I did sometimes read Google's AI overview to glean some basic information and Latex commands.

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7 APPENDIX

Heat energy Q , is the scalar product of mass flow, mass fraction w , enthalpy H .

$$Q = \dot{m} \sum_{i=1}^I w_i H_i$$

Where enthalpy is the integral of heat capacity with respect to temperature T .

$$H_i = \int_{T_{\text{ref}}}^T c_{pi} dT$$

Each physical property, of each molecule, in each temperature range has vectors C , and P . They are combined with a symbolic temperature T , to form the function

$$f(T) = \sum_i C_i T^{P_i}.$$

Which is used directly to represent quantities: isobaric, specific heat capacity c_p , thermal conductivity k and dynamic viscosity μ . However, a non-constant c_p cannot be used directly in heat balances, as this would violate the first law of thermodynamics. To do this, c_p must be integrated with respect to temperature, which is best done by applying the Fundamental Theorem of Calculus

$$\int_{T_{\text{ref}}}^T f(\tau) d\tau = F(T) - F(T_{\text{ref}}).$$

The antiderivative, which this theorem relies on, is obtained by:

$$F(T) = \sum_i \begin{cases} C_i \ln(T), & \text{if } P_i = -1 \\ C_i \frac{T^{P_i+1}}{P_i + 1}, & \text{otherwise} \end{cases}$$

and the enthalpy is obtained by evaluating the antiderivative at the symbolic temperature and some reference temperature:

$$H = F(T) - F(T_{\text{ref}})$$

Which was heavily used throughout the project. In the cases where there are segments of temperature ranges, the function segments f_i becomes the piecewise-continuous function:

$$g(T) = \begin{cases} f_1(T), & \forall T \in [T_{\infty}, T_1) \\ f_2(T), & \forall T \in [T_1, T_2) \end{cases}$$

and its antiderivative is likewise defined, but to use the enthalpy one must include the discrepancy between the function segments at the intermediate temperature T_1 . If reference temperature is below the intermediate temperature $T_{\text{ref}} < T_1$, enthalpy is:

$$H = \begin{cases} F_1(T) - F_1(T_{\text{ref}}), & \forall T \in [T_{\infty}, T_1) \\ F_2(T) - F_2(T_1) + F_1(T_1) - F_1(T_{\text{ref}}), & \forall T \in [T_1, T_2) \end{cases}$$

Conversely, if $T_{\text{ref}} > T_1$, enthalpy is:

$$H = \begin{cases} F_1(T) - F_1(T_1) + F_2(T_1) - F_2(T_{\text{ref}}), & \forall T \in [T_{\infty}, T_1) \\ F_2(T) - F_2(T_{\text{ref}}), & \forall T \in [T_1, T_2) \end{cases}$$

The data for most the species' isobaric specific heat capacities were obtained from appendix B of a Swedish bachelor's thesis [13]. However, the coefficients give the molar heat capacities [J/(mol K)], but they label them incorrectly as kJ/(kg K). It was rectified by dividing all coefficients by the molar mass of the specie. The remaining data was obtained from the following links [14][15][16][17].

