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Mathematical modelling of Degussa Furnace

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Abstract

The energy demands in the world is rapidly increasing and with this, a supply nuclear power is of much interest. Nuclear fuel is relatively efficient when comparing to power sources like wind- and hydropower plants. Pellets are used as fuel by many plants however, its main concern is to find maximize cost efficiency and minimize fuel-waste. Studying how to get the pellets to be as optimal as possible is of massive importance and in huge focus in order to match the worlds power demand.

These pellets are sintered in a furnace type known as ”pusher-type” furnaces that functions continuously and is incredibly efficient when it comes to its heat transfer capacity and high-performance output. In this sintering process, a gas-flow from the opposite side from the pellets interacts with the solid pellets in order to get the desired reaction. However, the turbulence and the nature of the multi-phase flow problem causes many unknown interactions and the main focus is do create a theoretical model based on the process parameters to understand what is happening in the furnace.

In this study, a simplified model of the inside of the furnace chamber was created in order to observe where and when in the furnace a dissociation from CO_2 to CO + O_2 would occur. Data given by Westinghouse was put into a mathematical model created in MATLAB and parameters given by the thermodynamic model was in turn put in to ANSYS, a program based on Computational Fluid Dynamics for a simulation. The simulation was considered a success when the gas-mix goes from 3% CO_2 to 0.4%. The CFD of the model estimates this to happen at 250 seconds, where as the thermodynamic model predicts the exchange time to be about 200 seconds. This study is a major first step in understanding the dynamics of the furnace.

Keywords

Furnace, CFD, ANSYS, Thermodynamic model, Exchange time

Sammanfattning

Energibehovet i världen ökar snabbt och då blir ett stadigt tillförsel av kärnenergi mycket intressant. Kärnbränsle är relativt effektivt jämfört med kraftkällor som vind- och vattenkraftverk. Pellets används som bränsle av många kraftverk och då blir det ett upphov att hitta maximal kostnadseffektivitet och minimera bränsleavfall. Att forska fram till hur man gör pellets så optimala som möjligt är av enorm betydelse och i stort fokus för att matcha världens energi behov.

Dessa pellets sintras i en ugnstyp som kallas ”pusher-type” ugnar som fungerar kontinuerligt och är otroligt effektiva när det gäller dess värmeöverföringskapacitet och högpresterande effekt. I denna sintringsprocess startar ett gasflöde från motsatt sida från pelletsen med de fasta pelletsen för att få den önskade reaktionen. Det blir ett flerfasigt flödesproblem och orsakar många okända interaktioner och huvudfokus är att skapa en teoretisk modell baserad på processparametrarna för att förstå vad som händer i ugnen.

I denna studie gjordes en förenklad modell av ugnskammarens insida för att observera var och när i ugnen en dissociation från CO_2 till CO + O_2 skulle inträffa. Data från Westinghouse placerades i en matematisk modell skapad i MATLAB och parametrar som gavs av den termodynamiska modellen lades i sin tur till ANSYS, ett program baserat på Computational Fluid Dynamics för en simulering. Simuleringen ansågs vara färdig när gasblandningen går från 3% CO_2 till 0,4%. CFD:n för modellen uppskattar att detta händer vid 250 sekunder, där den termodynamiska modellen förutspår utbytestiden till cirka 200 sekunder. Denna studie är ett stort första steg för att förstå ugnens dynamik.

Nyckelord

Ugn, CFD, ANSYS, Termodynamisk model, Utbytestid

Contents

1 Introduction

1.1 Background

To meet the increasing energy demand with a sufficient supply nuclear power technology is of particular interest, nuclear fuel is comparatively effective regarding renewable energy sources such as hydropower plants and wind turbine power. The main concern of nuclear power generation using pellets is to increase the fuel burn-up to optimize cost and decrease waste of spent fuel. Fuel burnup is a measure of how much power the fuel has created and how much fuel has depleted [1]. It is therefore valuable to study the processing of nuclear fuel to possibly find ways to improve the performance of the fuels.

The main raw materials used for today's nuclear fuel is uranium. Uranium is relatively commonly occurring metal on earth, about as common as tin. After mining uranium, the ore is crushed and treated with acid or alkali which results in yellow cake with the composition U_3O_8 in powder form. The yellow cake is then converted into the uranium hexafluoride UF_6 and is then shipped off to enrichment plants. Natural uranium is usually found in the two isotopes 238U and 235U, in the enrichment stage the UF_6 is enriched with the desired isotope of uranium 235U by inserting the gas in a centrifuge where the heavier isotope 238U is pushed to the wall and the 235U enriched gas is then extracted, the gas is then converted into powder UO_2 which is then sintered [2].

The sintering process increases the grain size of the pellets and closes pores in the material. The pellets are then loaded into fuel rods and assembled to fuel cells which are finally manufactured to the power plants. The pellet sintering process is done in a Degussa oven that reaches high temperatures around 1625-1780 °C in a hydrogen gas atmosphere. The containers holding the pellets referred to as boats need to resist high temperatures, these boats are usually made from Molybdenum, other materials such as TZM, a titanium zirconium molybdenum alloy for example, has also been used [2].

Westinghouse Electric Company is a manufacturer of nuclear fuels and other services regarding nuclear power plant logistics. The fuel operations department situated in Västerås; Sweden distributes fuel cells to various plants in Europe [3]. In their sintering furnace where the boats loaded with the UO2 is pushed in, a counter current of hydrogen gas mixed with a small amount of CO2 is present. This gas has several functions, the hydrogen gas protects the metal parts of the furnace from contacting air, eliminates the lubricant added to the UO2 in preparation of sintering. The gas also helps distribute and remove heat uniformly [4].

1.1.1 UO2 Sintering furnace

The sintering furnace is known to be a MOX model, one of the first to ever be produced was from the Degussa Company. Degussa, after a long time became ALD France after over 100 years. Together with their parent company that focuses on vacuum technology, ALD France further developed their sintering furnace based on the earlier MOX-model to guarantee quality fuel production to its customers. These furnaces in question are specifically engineered to efficiently sinter UO2 fuel pellets.

There are multiple things that make these furnaces so incredibly useful for the companies that use them. One is that they are “pushers-types”, as seen in figure 1.1. A pusher-type furnace is a furnace that can function continuously and is commonly indicated by its extreme heat transfer capacity and high-performance output. [5]. This guarantees a high reliability and assures high quality and efficiency. All this plus the low necessity of manpower and straightforward automation makes this a very inexpensive process [6].

1.2 Social and Ethical aspects

Nuclear power has always been an interesting and controversial topic amongst people and governments, especially considering how important the power source is in certain places in the world. Also, now that the fight towards climate change is at its peak, to streamline such an important aspect of nuclear power

to be as resource- and energy efficient as possible is a very high priority, for the environment and company resources.

Improving and streamlining this process will yield more and higher quality nuclear fuel that is important for the future fight to climate change. This will further evolve the nuclear power industry and will allow resources to be used more efficiently and significantly lower the energy costs to run the process.

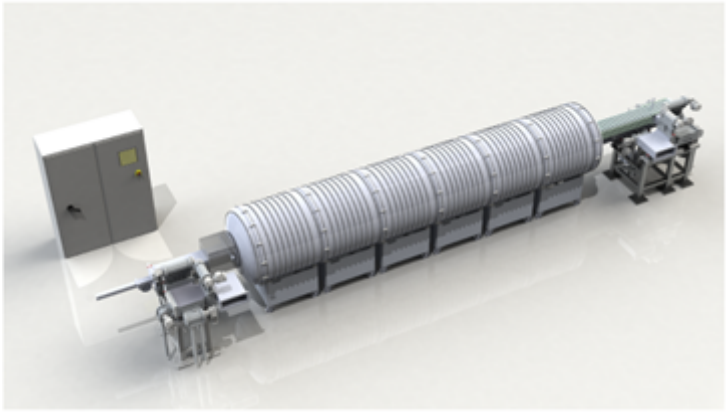

Figure 1.1: 3D-model of a UO2 sintering furnace (ALD France) [5]

1.3 Problem

Since the sintering furnace reaches extreme temperatures, it is very difficult to analyse what is happening in the oven during this situation. The gas-flow is single phase, solid material, including boats can be considered for at multi-phase flow problem. The complexity lies in the gas/solid interaction or gas mix. Can a theoretical model based on the process parameters be created to understand what is happening in the furnace?

1.4 Purpose

The purpose of this report is to analyse the transport phenomena critical parameters of the furnace and reproduce a system model of interest for Westinghouse Electric Company. The model is supposed to give insight on the phenomena that is happening in the oven with theoretical knowledge. To understand whats happening in the furnace, the following is suggested:

- Estimate heat-flux in and out out of the furnace based on a thermodynamic analysis.
- Investigate kinetic effect with a CFD model.
- How will the gas change throughout the furnace in the given conditions?

2 Heat and energy balance model

2.1 Energy balance

Specific heat capacity shows the amount of energy required to raise the temperature of a substance per mass unit. In SI-units, specific heat capacity is the amount of heat required to raise 1 gram of mass by 1 kelvin which is expressed as J/kg·K. Using the specific heat capacity of any given substance, one can calculate the energy required to heat up 1kg of mass to wanted temperatures. Since specific heat capacity is per unit mass, the value never changes, no matter the size of the system [7].

$$E = m \cdot C_p \cdot \Delta T \tag{1}$$

E stands for the amount of energy required, m is mass, C_p being the specific heat of the substance and ΔT stands for the temperature difference.

2.1.1 Enthalpy

Related to specific heat and the process, enthalpy shows the amount of heat transferred to a system at constant pressure. The enthalpy is calculated in a similar way and both these methods are an application of the conservation of energy and mass [8].

2.2 Combined law of thermodynamics

In thermodynamics, something known as Gibbs fundamental equation describes an equation that is the result of the first and second law of thermodynamics also known as the combined law of thermodynamics. Thermal dissociation is a reaction that is affecting the process and to thoroughly calculate and simulate said reaction, the combined law of thermodynamics is used. Besides dissociation, this law can be used for looking at a body where the volume varies with no flows of particles affecting the body [9].

2.3 Conservation of mass

The law of Conservation of Mass says that mass can neither get destroyed nor created. The mass will be conserved in its domain. When it comes to fluids, to be conserved, they must move in certain ways for there is no increase or decrease in mass. Given the density, volume and the area of the system, the amount of fluid in said system can be calculated [10].

$$E = \rho \cdot V \cdot A \tag{2}$$

ρ is the density, V is the volume and A is the area. The equation above states that the velocity of any area of the system can be calculated if the velocity is defined at any known area.

2.4 Courant number

The Courant number is a non-dimensional number that is often used in CFDs that gauges how fast information crosses a computational grid cell in each time-step.

$$C = \frac{u \cdot \Delta t}{\Delta x} \tag{3}$$

where C is the Courant number, u is the travel speed of the information, Δx is the grid cell and Δt is the time-step.

Choosing a Courant number greater than one will make the information spread to more than once cell per time-step and will result in an inaccurate solution. The information can “skip” cells and will result in missing answers and wont be able to converge properly. This can also lead to complex solutions that deviates from the desired physical results. In other words, a high Courant number will not be able to accurately explain the physical incident [11].

3 Method

3.1 ANSYS

The software ANSYS will be in focus this study. ANSYS is a software based on Computational fluid dynamics (CFD). CFD is a tool used to simulate the behaviour of fluid flows using numerical solution methods. Complex problems involving fluid interaction can be extremely hard to predict and analyse, however with CFD, it gets a lot easier. It is something that is used in many industries that work with aerodynamics and hydrodynamics as well as multiphase flows and so on to optimise and analyse product ideas before prototype phases. The fluid dynamics in question are primarily in the form of partial differential equations. The most important purpose with CFD is applying it in cases where using conventional calculations to analyse complex systems just is not enough. The subprogram ANSYS Fluent is a part of ANSYS that focuses on flow and fluid dynamics and will be used the most this study. This is a versatile software that contains the capabilities required to model and calculate the model flows and turbulence that will occur in this study [12].

3.1.1 Geometry

The geometry was acquired using a 3D-computer-aided drawing program or CAD. The modeler in this case was used to easily draw the model given the parameters given by data and the one model in question was sketched. It is a relatively simple yet efficient design. There are seven “major” zones in the chamber as seen in figure 3.1. These zones was divided into 11 more concise zones to further illustrate the different conditions inside. The finished and simplified model is illustrated in figure 3.2 and so is the gas flow.

3.1.2 Mesh

The meshing is the start of a process to achieve accurate results. Depending on the mesh placement and size, the accuracy is different for the flow of the matter affects the certain areas differently. Angles are inconsequential to an extent because of the straight nature of the mesh. Small elements will give a more time-consuming

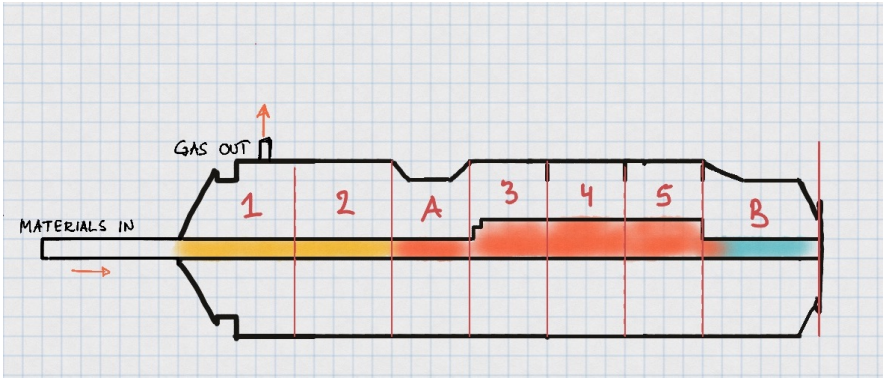

Figure 3.1: A simplified drawing of the furnace, it is divided into several zones named 1-5, A and B.

Figure 3.2: A simplified model of the furnace however, this one is divided into 11 zones

simulation and can be a cause for failure or a discrepancy in the result. The optimal result is given from a proper balance of time and precision, any disruption will sway this balance.

3.1.3 Governing equations

The governing equation for the conservation of a mass for a transient flow in i ($i = x, y, z$) direction is as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{4}$$

where ρ is the density and u_i the velocity vector component in the i-direction. The conservation equation of momentum in i ($i = x, y, z$) direction can be expressed by the following equation:

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho g_i \tag{5}$$

where ρ and μ are the density and viscosity of the liquid and gas phases and g_i is the gravity in i-direction and μ_t is the turbulent viscosity, which has different

expressions depending on what turbulence model is chosen.

The energy equation is based upon the first law of thermodynamics.

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot \left(\vec{u}(\rho E + p)\right) = \nabla \cdot \left[(\kappa_{eff} \nabla T) - \sum_j h_j \vec{J}_j + (\bar{\bar{\tau}}_{eff} \cdot \vec{u}) \right] + S_h \quad (6)$$

where κ_{eff} is the effective thermal conductivity, controlled mainly by the turbulence. $\vec{J}_j$ is the diffusion flux of species j. The total energy is treated as

$$E = h + \frac{p}{\rho} + \frac{u^2}{2} \quad (7)$$

where h is the enthalpy, p is the pressure, rho is the density and u is the velocity vector.

The scalar transport of a scalar Y_i is conserved in the equation:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot \left(\vec{u}(\rho Y_i)\right) = -\nabla \cdot \vec{J}_j + R_i + S_i \quad (8)$$

where R_i is the net rate of production of species i by chemical reaction, S_i is the rate of creation by addition from the dispersed phase plus any user-defined sources [13].

3.1.4 Initial and boundary conditions

• General: These are all the measurements and data given by Westinghouse that has been scaled and applied to both model and mesh. The measurements were all scaled to mm.

• Boundary conditions: The velocity of the incoming gas is constant throughout the model at 0.025 m/s. The gas is assumed to have ideal conditions. Two user inputs were also made, one at 97 and one at 3 representing the percentage of the carbon dioxide in the gas. Diffusion coefficient was put in at 900K, which

is considered to be the average temperature of all the zones.

3.1.5 Temperature profiles

The multiple zones in the furnace all have different temperatures and even if the temperature is the same in certain zones, there are several where the temperature is accruing. In the eleven different zones, there are five temperature profiles put into the ANSYS setup. The temperatures are assumed to grow linearly to get a profile that not only suits the model but also to get rid of deviations in the simulation that can lead to aborts. As seen in figure A.2 the profiles have a linear change depending on zone and the constant temperature were put into the other zones. Figures A.1, A.2 and A.3 all illustrate the same information but in different ways. A.1 and A.2 is more simplified and A.3 is the one showing temperature evolution in the zones.

3.2 Assumptions

There are several properties and certain models that were assumed before the mathematical model and simulations were made. For instance, the properties of the carbon dioxide in the production gas were assumed to function in ideal conditions. The geometry of the furnace was also incredibly simplified as the simulations show the fastest, most efficient way for the gas to react.

4 Results

4.1 Results from the mathematical model

Using the governing equations in 3.1.3 and the data given by Westinghouse Electric in a analytical model made in MATLAB, the mathematical model gives the absolute shortest time to exchange the gas to be 250 seconds, which is just over four minutes.

4.2 Results of the convergence

Multiple plots ran to reach a proper convergence of the simulation and to achieve a precise result. The plots ran along multiple residuals; x-velocity, y-velocity, z-velocity, K, Epsilon, energy, and continuity. These can be seen in figure 2, where the values of these residuals can be seen on the y-axis and iterations on the x-axis. To make certain of a fairly accurate result of the simulation, the residual should achieve a minimal value.

When it comes to the diffusion of the 3% CO_2 gas to 0.4%, figure 4.1 illustrates the process in an x/y-plot where the incline shows the diffusion in real time from the above portion being 3% going down to the lower section that is 0.4%. Observe that the x-axis is to be interpreted from right to left as it reflects the positions of the in- and output. The process takes approximately two minutes to react and reach the desired results.

The systems contour plot, figure 4.2, shows where in the simulation the diffusion happens and where the fastest point is. As the gas traverses through the mesh, a point will be created at the absolute front of the gas. It forms a point to show that the middle part is the fastest and the sides are slowed down by the walls of the chamber. The “empty” part on the left of the chamber is the 3% proportion of the gas and the final section at the far right is the 0.4% that was desired.

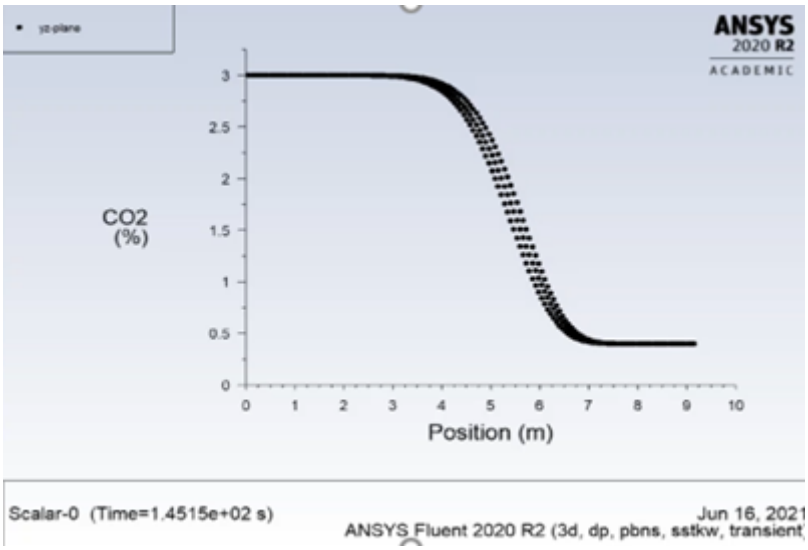

Figure 4.1: x/y-plot illiustrates the exchange rate happening inside the furnace

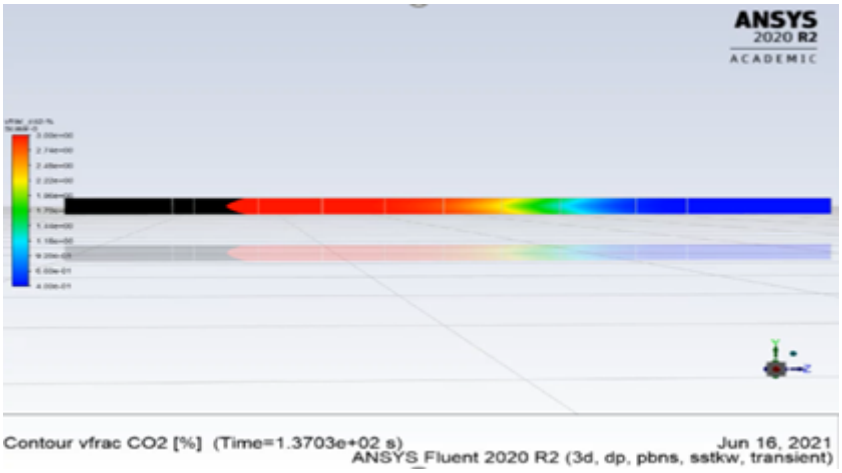

Figure 4.2: Contour plot of 4.1 and shows fastest point of the gas

5 Discussion

5.1 Discussion of the Thermodynamic model

The results of the thermodynamic analysis was primarily seen as a reference for the furnace and was done without any consideration of transient effects. This means that the model is of a progressive nature rather than a conservative measure. This model was primarily made only to get a ideal, optimal view of what was going on in the furnace and the results acquired were used as boundary conditions for the later stages of the study. The only part that could be ”improved” would be the accuracy and the volume of data. To get better boundary conditions for an accurate simulation in a functioning analysis would be the data that was given from Westinghouse. This data was, because of obvious reasons, altered. Although the boundary conditions from this model are accurate, only the employees of Westinghouse Electric know how realistic this is.

5.2 Discussion of the simulations

The CFD model of the DeGussa furnace was made to refine the progressive estimate of the gas exchange in the furnace. The CFD showed how fast the gas exchange would occur however, there are multiple factors that incredibly simplified this model and could potentially produce more accurate answers in the future.

A starting point would be to have a more accurate model. The models purpose was to produce parameters that would eventually be used as boundary conditions for the simulations. More precise boundary conditions would reflect more accurately on the real-life conditions and will produce a more refined model to simulate. A suggestion here is the data provided by Westinghouse

Another major aspect would be the geometry. The geometry illustrated in Figure 3.2 is incredibly simplified and highly resembles that of a duct with a square cross-section. There are multiple different geometries that make up the zones with different dimensions to roof, wall and bottom. The inlet and the outlet are in the model as large as the rest of the chamber which is very inaccurate and should look more like the ones in Figure 3.1. Besides the parameters, the geometry should be

a top priority to improve in order to get a more realistic model.

The CFD calculated a model that was assumed to be empty (besides the gas), this is not the case in real life. The said gas is constantly reacting to molybdenum boats filled with pellets that continuously gets ”fed” into the chamber. Apart from the reacting pellets, there will be a large amount of gas in the boats that will greatly extend the reaction time. As for the gas, the attributes are very simplified and the proper mix is needed to properly simulate the diffusion and when the gas dissociates.

6 Conclusions

In this work, to accurately depict and replicate a real-life sintering furnace, multiple steps has been presented and analyzed. This was done in two stages, a thermodynamic analysis and a CFD simulation. To summarize, the findings were;

- A thermodynamic analysis of the DeGussa furnace was done in Matlab. The outcome is a reference for the furnace without consideration of transient effects and are thus of a progressive nature rather than a conservative measure.
- In addition, a CFD model of the DeGussa furnace was done that refines this progressive estimate for describing the process gas change in the furnace. This is a first step at understanding the dynamics of the furnace.
- Specifically, the thermodynamic model predicts an exchange time of about 200 s, whereas the CFD model estimate it to 250 s.
- Overall, a first step in understanding the DeGussa sintering furnace has been achieved.

7 Future Work

To improve upon these simulations, a good place to start would be the geometry. As seen on (hand drawn picture), the zones are not equal in shape as they are in the model, even though the length of said zones are the same in the model. One of the things to change in that regard is to make sure that the walls of the warm parts or zones would be higher which will lead to high and different ceilings. Another this is that the in- and outlet is in other areas of the modelled furnace. Not only are they a lot smaller in size, but they are also located on the "roof" of the furnace. A change in size would lead to a change in pressure whenever the gas enters or leaves. To have an inlet as large as the chamber does give the fastest, most optimal result but it is not at all realistic.

When it is time to finally simulate with the filled molybdenum boats, a consideration would also be to mind that the boats have a large amount of gas in them besides the uranium dioxide that would extend the reaction time.

Figure A.4 shows the energy change per zone while considering the boats and could be a good place to start when doing this project in the future.

The attribute of the gas is also very simplified as mentioned before and is to take into consideration if the gas is to gain different properties depending on the degree of mixing of CO_2 as well as when it dissociates to $CO + O_2$.

When it comes to the temperature profiles, the biggest interest would be to reconsider the degree of temperature change. The profiles are assumed to have a linear growth throughout the zones until it reaches the desired temperature however, exactly how the temperature changes are unknown. Maybe adding multiple degrees in the polynomial could more accurately describe the temperature changes.

8 Acknowledgements

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Appendix: Temperature graph

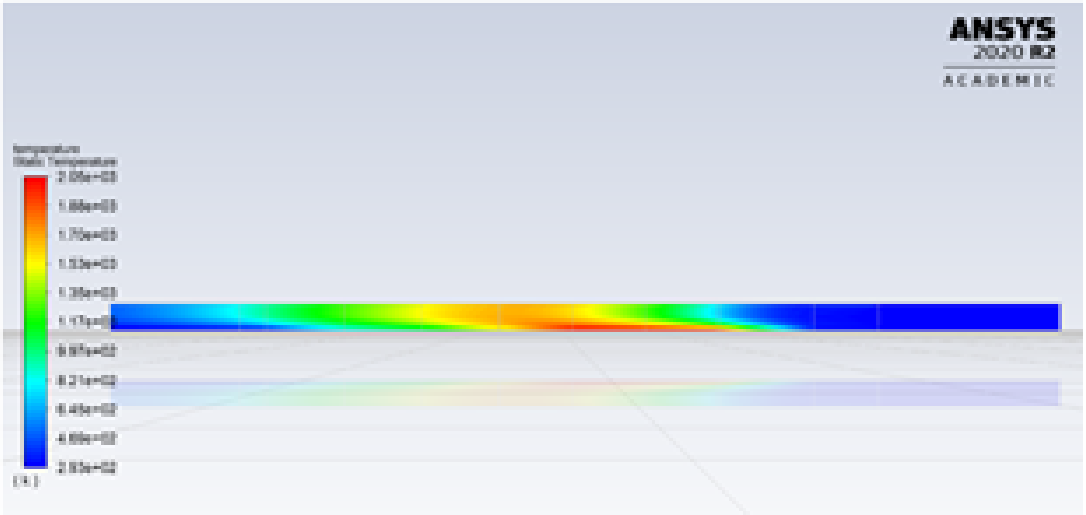

Figure 9.1: Shows where in the chamber the gas is at its hottest

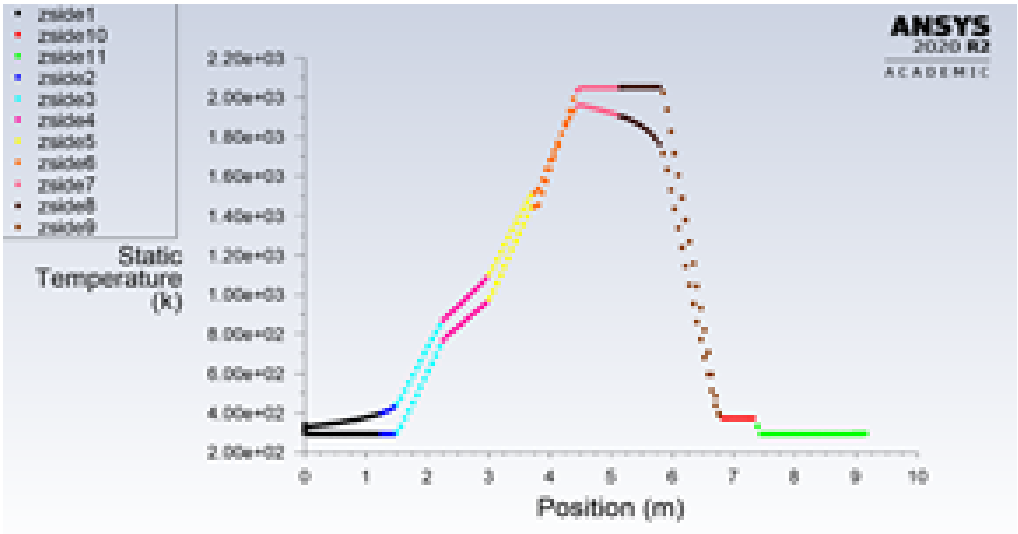

Figure 9.2: Shows the temperature changes relative to zone/distance

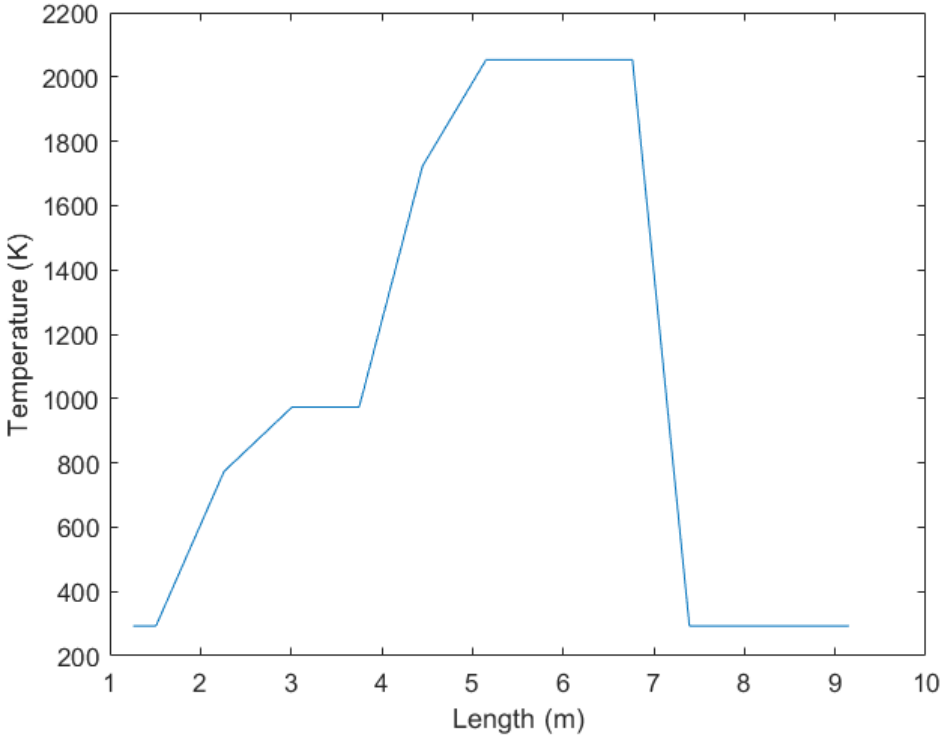

Figure 9.3: Shows temperature relative to graph

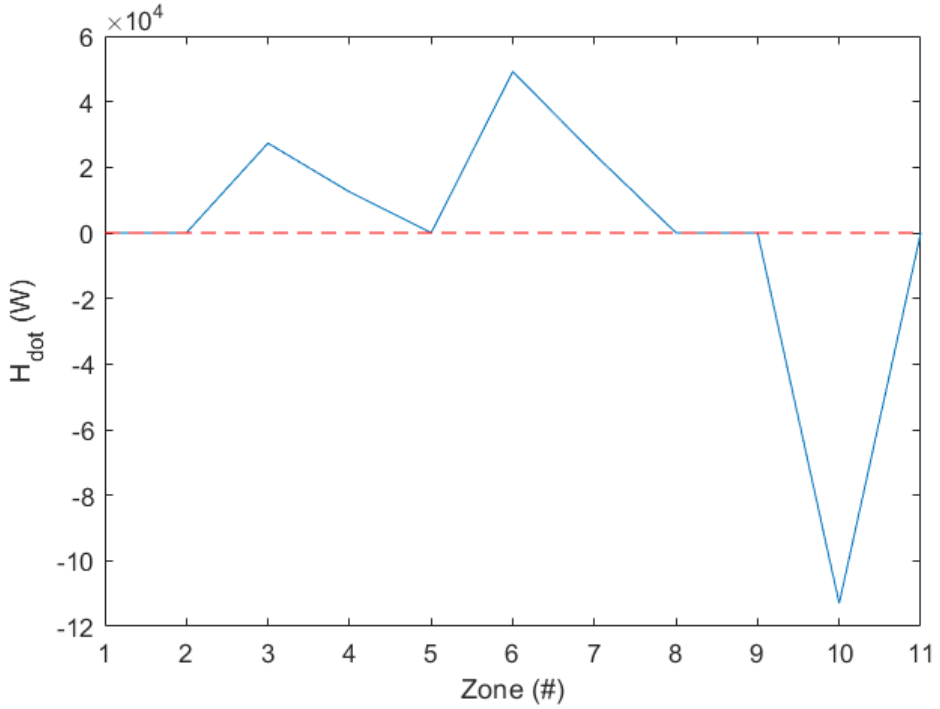

Figure 9.4: For future work, shows the change of energy at a certain zone with molybdenum boats

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