CFD Simulation and validation of downdraft Pottery Furnace
Numerical Study of Heat and Mass Transfer Phenomena, Radiation and Evaporation

Master of Science Thesis

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CHALMERS UNIVERSITY OF TECHNOLOGY
Göteborg, Sweden, 2012
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Cover:
Picture of an old traditional Indonesian updraft kiln during loading

Göteborg, Sweden 2012
Abstract

Pottery is an important industry in Kasongan, Indonesia, and they export their products all around the world. However, their kiln, a ceramics furnace, is undeveloped and they have problems with the quality of the product since the ceramics does not reach the vitrification temperature of 900°C which is needed for the best quality. Therefore, students from University Gadjah Mada, Yogyakarta, and Chalmers University of technology, Göteborg, have been trying to develop the kiln with the help of simulations and this have resulted in a new design where the flue gases will pass the ceramics downwards instead of upwards. The purpose is to continue the simulations and validate the simulations with the new kiln in order to continue the development.

The simulations was done with computational fluid dynamics with models for turbulence, energy, radiation, and water evaporation with a specific heat capacity change. The idea was to get good enough simulations to directly comparison with measurements, but the kiln was never built during the project and no measurements were obtained. Thus, important measurements as inlet temperature and flow and amount of ceramics are not available and the values was approximated instead. The inlet temperature was assumed to 1000°C, the inlet flow was calculated to be able to evaporate the water and heat the ceramics 800°C and the amount of ceramics was assumed from other measurements.

The mean temperature of the ceramics only reached 404°C and the minimum temperature of the outer surface was 339°C, the ceramics did not reach the vitrification temperature, and the approximations was probably underestimated. The inlet velocity was probably too high since it created a big swirl that pushed all heat into the opposite corner, this could be tracked with both the temperature distribution and the velocity profile.

Despite the assumptions and mesh dependency, it is probably possible to use the models for the development of kilns since it is reasonable to assume that the errors would affect different design in the same order of magnitude. It might also be possible to simulate temperature distribution, and therefore kiln efficiency, with the velocity profile, which would decrease the computational time a lot.
Acknowledgement

First, I would like to say that I am very grateful that I got the possibility to work with such a fun and interesting project like this. I also want to thank Gadjah Mada University, Yogyakarta, Chalmers Vänner and Chalmers MasterCard for their financial support, it would have been much harder without it.

I would like to thank Professor Bengt Andersson for his great source of knowledge and ideas and his help in this project. Thanks to my supervisor Professor Rahman Sodiyo at Gadjah Mada University for his help in Yogyakarta with this project.

Also big thanks to Mr. Dedi Eko, not only for his practical help with everything in Yogyakarta, but also for his friendship. Without him, the days at the office would have been much longer.

I am also grateful to all new friends in Yogyakarta that showed me Yogyakarta from its best side and for their hospitality. Special thanks to Helena and Raja for your company and dinners, and for finally have someone to experience that amazing country with.

I also would like to say thanks for the everlasting support from my family and friends and all love to Johanna, for her encouragement and that she always bring out the best of me.
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1 Introduction
In Indonesia, pottery production is an important industry, both socially and economically, and the traditions devolve from generation to generation with trial-and-error developments mostly. The pottery fires in an updraft kiln, a ceramic furnace, and they have problem with cracks in the pottery and they do not take any measurements during the firing process.

1.1 Background
To improve the firing, cooperation between University Gadjah Mada, Yogyakarta, and Chalmers University of technology, Göteborg, is established and during the years students have developed a model for simulation with computational fluid dynamics, CFD, and a new kiln plans to be built in Kasongan, with improvements from the work (1) (2) (3). The big difference is that it will be a downdraft kiln and the fuel will change from wood to briquettes made of coconut shells. There are a few downdraft kilns in the area, but they are not in use due to very long cooling period and they are harder to operate with the consequence that the roof almost blew off one of the kilns.

The purpose is to continue develop the kiln and this will mainly be done in two ways, validation of the simulations and the models with the new kiln and making new proposals to improvements from new simulations. It is also of interest to investigate how the fuel change from wood to coconut shell briquettes is accepted, worked out and how it affects the kiln and its performance.

If the pottery makers accept the new kiln and keep using it, the product will probably be of a better quality that would increase the profit both in short and long terms. Hopefully the kiln is good enough so more kilns of this design is produced and the use coconut shell briquettes increase and thus, leads the society in a better direction economically, socially and environmentally.

1.2 Objective
The objective is to simulate a kiln with the size of the planned kiln with the CFD models developed by the research and investigate the effectiveness and its limitations. Representative measurements in the new kiln are to validate the models and to see how good the simulations predict the reality. There will also be measurements to confirm the inlet and boundary conditions to the simulations and to determine how good the firing of the ceramics is.

It is also of importance to evaluate the usage of the coconut briquettes, since the potters often want to keep their old traditions. The cultural difference might also lead to unexpected difficulties to perform the validation and to the work in Yogyakarta.

The new design has to be feasible in Indonesia, which implies material limitations, an eventual constrain from the potters for non-traditional kilns and the energy source has to be the best from an Indonesian point of view, both environmentally and economically. The equipment to validate the kiln either has to be available in Yogyakarta or transported to Yogyakarta, both for a low cost. Thus, only usage of simple equipment is feasible.
2 Theory
The readers that are not familiar with CFD and firing ceramics can find the help in this section. First, it is about traditional production of pottery with the main step and concepts and a description of what happens with ceramics during heating, all to understand how pottery ends up as it does. The second part is fundamental theory about the method for the simulations, computational fluid dynamics (CFD). The method is very software specific and the last theory part is to introduce the reader to the software.

2.1 Clay
Clay mineral is aluminosilicates that consists of alumina, \( \text{Al}_2\text{O}_3 \), and silica, \( \text{SiO}_2 \), and the clay in the pottery for this case is a mix of kaolinite and halloysite and 20% of the dry content is sand and the other 80% is clay. (4) The structure consist of layers, where there is one of silica and one of aluminium and between them, there are layers of oxygen and hydrogen that is the chemically bounded water in the clay, see Figure 1. (5) Both kaolinite and halloysite have the same chemical formula, \( \text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 \) and belong to the kaolin group, where the difference between the materials are how the layers are stacked and that the halloysite is hydrated with two water molecules. (6)

![Figure 1 Structure of Kaolin (5)](image)

2.2 Traditional production of pottery
Pottery starts with mixing of clay, sand and water to achieve the desired plasticity, in order to shape the pottery without a shape change afterwards. It is important to get a homogeneous mixture, otherwise it might crack and the quality might be uneven. When the potteries have the desired shape it need to dry and this takes a few days dependent of if it is dry or wet season. The dry but not fired pottery is a green body. It is important not to dry it directly in the sun, because then it will go too fast, since the evaporated water will not be able to transport out of the pottery, and it will crack. (4)
The green body is ready for firing when most of the unbounded water evaporated and the water content is in equilibrium with the air. The traditional kiln used in the villages around Yogyakarta is an updraft kiln, where the flue gases is going upwards in the chamber. The flue gases are lead through holes in the floor to the pottery, up through the chamber and exit at the roof of the chamber. Straw and a layer of tiles are covering to prevent the flue gases to exit too fast. The new kiln will instead be downdraft, where the flue gases will transported to the top of the chamber, go down through the pottery, out of the holes in the floor to a nearby chimney. The roof is made of bricks, the same material as the rest of the walls. The chimney will make a under pressure since the flue gases will rise in the chimney due to a lower density and that will drag the flue gases through the chamber to the chimney.

The downdraft has one advantage than the updraft. When a cold space of flue gas somehow emerge in an updraft kiln, the gas will get a higher density and its speed through the kiln will be retarded and will then push the following hot flue gases to take another way. For the same case in a downdraft kiln, the increase in density will just make the cold gases pass faster through the kiln and new hot flue gases can obtain its place. This will make the temperature distribution in the kiln more even.

To be able to load the kiln with pottery, traditionally a part of a wall of the kiln is "loose", that one is taken down and after the kiln is loaded the wall are closed again. The new kiln will instead have a door. During the loading, the main target is to get as much pottery into the kiln as possible. The potteries size can vary from two decimetres to two meters and the small potteries are placed in the gaps between the bigger ones, all unstructured.

In the beginning of the firing process, the preheat period, the fire is kept just outside of the inlet with low amounts of fuel put on the fire to heat the kiln at a slow rate, this usually takes three to four hours. Traditionally a kiln has two inlets, the new kiln will also have two inlets but it is uncertain if both will be used. The amount of fuel added will then increase and potters push the fire further and further into the inlet. During the fifth or sixth hour, they put wet straw on the top of the roof to prevent flames to burst out from the kiln. They will eventually turn into a fine grey ash and that usually indicates that the firing is finished. The ruling to finish is if the ceramics have started to glow, then the fire allows burning out. The firing takes 6-8 hours, often during the day so the kiln can be left to cool down during the night and unloaded the next day.

### 2.3 Heating effects on ceramics

The firing process starts slowly and initially the unbounded water in the pores is evaporating, until all unbounded water is gone. During all the steps where water is evaporated it is important that the heating is slow, since if the evaporation is faster than the transport and diffusion out from the body, the accumulated gas will cause bubbles that might crack or even explode the ceramics.

It is not until 500 to 600°C that the bounded water will evaporate and the heating has to be slow so the gas can escape. At 573°C one of the quarts inversions occurs, where the structure of the silica oxide changes. The inversion causes the pottery to become 2% larger when heating and 2% smaller during the cooling where the structure is going back again. Due to the size change, the ceramics can easily crack during the inversion and the heating and cooling has to be slow through.

The next step to reach is the sintering temperature, with occurs around 900°C. Here the clay particles start to melt together due to the vitrification process that makes liquid glass that flows out into the
pores of the ceramics, which makes the pottery stronger. Different degrees of vitrification refer to different temperatures for different clays, with ranges from 900°C up to 1400°C. (5)

What happens in the clay can be seen from the shrinkage, as in Figure 2 where the shrinkage for the clay that is used in Kasongan is seen. The first dip around 100°C is for the last unbounded water, between 400 and 600°C is the bounded water evaporated, also known as the dehydration of kaolinite. Around 900°C and above 1000°C are the vitrification processes where the first one is the formation of spinel alumina (9) and the second one is the formation of mullite (7) and transformation of the remaining cristoballite. (4)

![Figure 2 Shrinkage and change of shrinkage over the temperature in degrees Celsius (4)](image)

### 2.4 Computational Fluid Dynamics

Computational Fluid Dynamics, CFD, is a very useful tool for chemical engineers with its ability to predict equipments quality and performance without having it in physical form, a so-called virtual prototyping. That is where the problem awaits, CFD is mostly only a prototype, predictions from models of reality, even with the best computers. (10)

CFD basically solves what comes in, out, accumulates, produces and consumes in a certain control volume, done numerically in an iterative way. Solving Navier-Stokes (NS) equations with the equation of motion and the continuity equation is CFD for a flow. This often gives accurate solutions for laminar flows since viscous forces is dominant, but for turbulent flows the length and time scales becomes too small to be able to accurately solve it for normal sized chemical equipment. Just a normal mixer with one litre of water would need 10 micrometer big cells and timescales of 0.1 milliseconds to be solved properly. Thus, models, assumptions and approximations needs to decrease the computational cost to give up the information that would have provided to the result. This compromise between computational cost and accuracy is always present in CFD simulations. (10)
2.4.1 Governing transport equations

The first assumptions for flow simulations are that the flow is incompressible. That implies that the density is constant along the streamline and that the equation of continuity can shorten to equation 2.1. The fluid in the flow also considers as a Newtonian fluid which most of the used fluid is, like water and gas. For a Newtonian fluid the viscous stresses is linear, thus the viscous stress can be simplified to equation 2.2. These two assumptions reduces the equation of motion to equation 2.3, and the terms physical matter from the left is accumulation, convection, pressure change, diffusion and last a source term. To discretize the problem, the geometry divides into cells that makes the partial differential equations to become algebraic equations, that leads to a numerical error is introduced that is smaller, the smaller the cells are. This adds to the compromise between computational cost and accuracy. (10)

\[ \frac{\partial u_j}{\partial x_j} = 0 \quad 2.1 \]

\[ \tau_{ij} = \tau_{ji} = -\mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad 2.2 \]

\[ \frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) + G_i \quad 2.3 \]

2.4.2 Turbulence modelling

Turbulence is an important property for chemical engineering since the natural chaotic behaviour increase the mass- and heat transfer, that most of the time is highly desired. There is no exact definition of a turbulent flow, but there are some characteristics. The diffusive property comes from the chaotic motion and that is turbulent eddies in various sizes, that is stretching and tilting in all three dimensions and causing the speed of the flow to be flocculating and irregular. The flow is unstable at high Reynolds numbers and so are the eddies that is produced, thus they break up to smaller eddies, transferring the energy to a smaller scale, to eventually die when the viscosity of the fluid becomes to dominant unless new energy is added. Turbulence is a continuum phenomenon that occurs in a scale much larger than molecules length scale, turbulence is also a property of the flow, not the fluid. (10)

Turbulence is due to the chaotic behaviour very computational expensive to predict, thus models and approximations simplifies the solution. Reynolds decomposition is a statistical method where the velocity divides into its mean and fluctuating part, equation 2.4 and the mean value is a time average equation 2.5. (10)

\[ U_i = \langle U_i \rangle + u_i \quad 2.4 \]

\[ \langle U_i \rangle = \frac{1}{2T} \int_{-T}^{T} U_i dt \quad 2.5 \]
The turbulent kinetic energy, equation 2.6, can describe the intensity of the flocculation in the same way equation 2.7 describe the kinetic energy. The mean kinetic energy can then be decomposed as in equation 2.8 into two parts, one for the turbulence and one for the mean flow. The pressure decomposes in a similar way for compressible flows and thus the density needs to be decomposed.

\[ k = \frac{1}{2} \left( \langle u_1^2 \rangle + \langle u_2^2 \rangle + \langle u_3^2 \rangle \right) \]  

\[ E = \frac{1}{2} U_i U_i \]  

\[ \langle E \rangle = \frac{1}{2} \langle (U_i + u_i)(U_i + u_i) \rangle = \frac{1}{2} \langle (U_i)\langle U_i \rangle + \langle u_i \rangle\langle u_i \rangle \rangle = \bar{E} + k \]  

The models that use the Reynolds decomposition to solve the Navier-Stokes equation have a name: Reynolds Average Navier Stokes equations (RANS). For all those, equation 2.9 is a general writing of the Navier Stokes equation, the terms in order from the left is accumulation, convection, pressure change, diffusion and last is the Reynolds stresses. The Reynolds stresses contain the connection between the mean and fluctuating velocity field. In order to close the equation and solve it, modelling of some parts of the equation is necessary and that is the main purpose of RANS-modelling.

\[ \frac{\partial \langle U_i \rangle}{\partial t} + \langle U_i \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} = -\frac{1}{\rho} \frac{\partial}{\partial x_j} \left\{ \langle P \rangle \delta_{ij} + \left( \frac{\partial \langle U_i \rangle}{\partial x_j} + \frac{\partial \langle U_j \rangle}{\partial x_i} \right) - \rho \langle u_i u_i \rangle \right\} \]  

Many of the turbulence models use the Boussinesq approximation to model the Reynolds stresses. That is based on that the Reynolds stresses may depend on the mean velocity gradient, as in equation 2.4. It proposes that the transport of momentum by turbulence is a diffusive process, as if it behaves like molecules. If the details about the turbulence are not important, the fluid approximates as a pseudo-fluid with an increased viscosity, the eddy viscosity \( \mu_T \). This approximation has several limits due to the assumption about the diffusion behaviour that turbulence is isotropic and that local equilibrium exists between stress and strain.

Nevertheless, the eddy viscosity has to be determined and the turbulence models are often quantified by the way the eddy viscosity is modelled and how many additional transport equation that is needed to be able to solve the equations. Zero- and one-equation models are often too inaccurate to use for general-purpose flow simulations. Two equations considers to be the least number of equations to get an appropriate model since the length and velocity scales needs two quantities to be determine. Mostly, the velocity scale is determined by the k-equation (kinetic energy) and the length scale is determined by a property that is directly connected the length scale, the l-equation.

One of the most popular two-equation model is the k- \( \epsilon \) model, where \( \epsilon \) is the energy dissipation rate and the turbulent viscosity, \( \nu_T \), is \( \nu_T = c_k k^{3/2}/\epsilon \). It is a robust and easy interpreted model, but the standard k-\( \epsilon \) model is not always accurate. The standard k-\( \epsilon \) is not accurate with flows with streamline curvature,
swirling flows and axi-symmetrical jets and the inaccuracy derives from the Boussinesq approximation. The model derives to fit flows with high Reynolds number and the model is often too dissipative, thus it might have problem with areas of low Reynolds numbers. The RNG k-ε model has an additional source term in the ε-equations, which reduces the destruction of ε, thus it handles swirling flows and flows at geometries that have strong curvature better. (10)

2.4. Mesh
The meshing is one of the most important steps in the CFD process, too dense mesh and the accuracy decrease and too fine mesh the computational time increase. There are two kinds of grids, structured and unstructured, where the structured for three dimensions consist of hexahedrons (six sides) and the unstructured of prisms, pyramids, hexahedrons and tetrahedrons. Mostly, the structured mesh requires less memory, resolve faster and has better numerical properties than the unstructured, but the structured mesh is sometimes impossible or hard to obtain for complicated geometries. (10)

There are a number of qualities that can be measured in a cell to help the user to not obtain an inaccurate solution. Two of the more important are the orthogonal quality and aspect ratio. Orthogonal quality measure how much the cell differ from the optimal cell and aspect ratio measure how flat the cells are. There are no exact limits, but they can differ from case to case dependent of the required accuracy. The accuracy of the cells quality can also vary in the geometry, an example is that cells with worse aspect ratio can be accepted if they are along with the flow, since it will only be relatively small gradient is such directions. (10)

It is important to get a solution that is as mesh independent as possible. The inaccuracy is visible if the same problem solves with different meshes, where the one with smaller mesh size will be more accurate and show a different solution. This may occur from big gradients that need a smaller mesh to be resolved with satisfied accuracy and this is often fixed by adapt the mesh based of the most important gradients in the system. There will not be a perfect mesh since most of the physics are in molecular scale and small meshes like that are not efficient, but it is a matter of getting the mesh good enough so the there are no big differences. (10)

2.4. Reaction modelling
One important aspect of CFD for chemical applications is the reaction model. The evaporation of bounded water models with the laminar finite-rate model, thus it disregards the effects of turbulent mixing and the desorption, \( r_{des} \), determines by the Arrhenius equation 2.10 with an activation energy equal to the heat of evaporation. (11) It is considered as one back and one forward reaction, both surface-dependent, where the adsorption is the backward reaction dependent of the partial water pressure, equation 2.11.

\[
\begin{align*}
    r_{des} &= A_1 \cdot e^{-\frac{E}{RT}} \cdot \theta_{H_2O} \\
    r_{ads} &= A_2 \cdot P_{H_2O} \cdot (1 - \theta_{H_2O})
\end{align*}
\]

Where \( A \) is the pre-exponential factor, \( E \) is the activation energy and \( R \) is the gas constant, \( T \) is the temperature, \( \theta_{H_2O} \) is the surface coverage for the evaporation sites and \( P_{H_2O} \) is the partial pressure of water. (11)
2.4. Radiation model
The model for the radiation absorption in the porous ceramics and fire wall is discrete ordinates. Basically it solve the radiation transfer equation by turning it into a field equation for radiation intensity, equation 2.11, for a finite number of angels set by the user, with N equations and N unknowns. (11)

\[ \nabla \cdot (I(\vec{r}, \vec{s})\vec{s}) + (a + \sigma_s)I(\vec{r}, \vec{s}) = an^2 \frac{\sigma T^4}{\pi} + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(\vec{r}, \vec{s}')\Phi(\vec{s} \cdot \vec{s}')d\Omega' \]

2.11

The amount of energy that is absorbed sets by the absorption coefficient that will be determined for the absorbing parts of the kiln by a user-defined function, UDF. A UDF is an external code that written in C++ and then compiled or interpreted into fluent. The radiation for all other solid walls are modelled as blackbody radiation. (11)

2.5 Software theory
First, the geometry draws in a design program. An easy way to produce a three dimensional geometry is to extend areas into volumes. To separate different parts from each other, volumes subtracts from other volumes in a so-called Boolean operation. This creates only one surface between the volumes, compared with slicing that creates two surfaces. It is also common to perform this to divide the geometry in smaller parts to enhance meshing.

The next step is to create a mesh. The program allows the user to set up rules for the meshing algorithm and can decide easy and straightforward settings as cell size and number of cells between a gap, and settings that are more complex that changes the algorithm for different regions or the cells format.

In the simulation program, there are many settings to decide and keep track on. Before any setup, it is good to make an analysis of the mesh quality to avoid numerical errors. The setup is mainly two different parts, the problem and the solution setup. First, it is to decide whether it is a steady state simulation or if it is time dependent. Then there are different phenomena to include, such as viscous forces, energy, radiation and multiple species. Many of them also got different kinds of models that all differ in accuracy and computational time for each phenomena. There is also a material section to set what material to use and what properties they have. In the cell zone condition the properties for the different volumes are set, such as if it is a fluid or a solid zone and to specify where different phenomena is occurring, a good example is that a reaction might only take place in certain regions. Often the last part is to set up the boundary conditions, such as flow or temperature of the inlet and wall properties as the walls shear stress on the fluid or thermal properties both in and outside of the wall.

In the second part the settings for the solution algorithms is set. First, the solution method determines, deciding the algorithms working path through the mesh and how to handle an eventual time step. In the solution controls, the speed of the iteration decides for the different equations with under relaxation factors, where a value close to one solves fast but increases the risk of divergence and flocculation and a value close to zero make the solution more stable, but increase the computational time. The next part is monitors, where the settings for the residuals sets and eventual monitoring of different values are set, like a temperature in a certain volume or a flow through an area. All algorithms need a value to start calculation from, and that is set in the solution initialization or from earlier simulations if they might
provide well starting values. There is also the possibility to save data automatically during a simulation in the calculation activities section, where also settings for other activities like animation and case modification is set. The last part is to decide the time step and the number of iterations per time step for time dependent cases or number of iterations for steady state cases and then run the simulation. There is also a results part to display contours and calculate values or fluxes from the data.

The software provides a specialist vocabulary. They are important to describe the settings for the simulation and here follows a short introduction to the used methods in the meshing part. The first and most important are inflation, which implies that the number of cells inflates near a wall or other kinds of surfaces or lines, mostly to improve the accuracy near the walls where the velocity profile often changes a lot. Multizone is a method to select parts of the geometry and automatically decompose these parts into either a structured or an unstructured mesh. Hex dominant is partly a setting in multizone to fill an unstructured mesh with more hexahedrons. CutCell is a method to keep a structured mesh for geometries that is hard to mesh structurally, by allowing bigger structured cells to split up into smaller structured cells and therefore match a change in the geometry easier.

3 Method

The works started in Gothenburg, where the target was to gain knowledge of the CFD-software, make some literature research that might help in the decisions of the validation process, evaluate, and understand the simulations that resulted in the new kilns design. The work was then continued in Yogyakarta where the validation was supposed to be done and the simulations updated regarded to the measurements, but the construction of the new kiln was delayed and the measurements were never done. There was also supposed to be some new design simulations to develop the kiln, especially to investigate the design of the inlet and the firewall. In the end of the project, a small study visit to the ceramic kilns in Höganäs was done to compare the old Swedish kilns with the Indonesian to improve the design.

First, the method of the simulations are presented, where it is focus on the ability to reproduce the simulations and provide reliability. Thus, these parts contain a lot of software specific information and are hard to follow for readers without that expertise. The second part describes how the measurements of the kiln were planned to be performed.

3.1 Method and settings for the simulations

The main goal of the CFD simulations was to get a simulation so good that it was directly comparable to temperature measurements from the real kiln so the models could be validated. An underlying goal was to increase the knowledge of the process. The set of models and settings was taken from the last master thesis in the area of expertise made by Nilenius, 2011 (1), but some things was changed to fit the new kiln better and the models were updated during the project due to results from simulations. Thus, method and settings for the underlying simulations are presented first and the final method and settings are presented last. The files from the last simulations from Nilenius, 2011 (1), were available and used initially. A sensitivity analysis of the time steps, mesh and radiation has also been done.
Most of the software that was used for the simulations are included in the ANSYS 13.0, the geometry was built in ANSYS Modeller, the mesh in ANSYS Mesh and Fluent was used for the CFD calculations. MATLAB were used to calculate good approximations.

### 3.1.1 Discarded geometry and mesh

The dimensions of the kiln were the same ones that were used for building the new kiln, which will make them suitable to be compared. The kiln dimensions can be seen in Figure 1, there the thickness of the firewall, the wall that creates the inlet, is 65 millimetres, and all dimensions were decided by Professor Sudiyo (4). The pottery that is put in the kiln is often at different sizes, shapes, heights, some of them are hollow and others are not. The walls of the hollow pottery is often between two to three centimetres thick, which implies that if the size of the mesh would have been that small, the whole kiln of about 25 m$^3$ would be millions of cells, thus the mesh will have to be of different size for different places in the kiln. Add that the wall of the pottery also need about five cells to be able to handle the change of water content and temperature in the ceramics.

Initially the ceramics consisted of three pieces of square pots with 2.5 centimetres thick walls and around 40 boxes. Many different kinds of meshing methods where used to achieve good mesh to this, i.e. CutCell, hex dominant and multizone, all with an inflation to the pottery. But either the numbers of cells got too high, the quality of the cells too bad or the number of cells in the walls of the pottery to bad or few, mostly because of the small walls in the pot resembling ceramics. Thus, the ceramics were then modelled as 45 plain cubes with the size of four times four times three decimetres.

The meshing for the cubes was done with advanced size function on both proximity and curvature, relevance centre on fine, average size of five centimetres. The number of cells across a gap was set to one since the firewall would be overcompensated otherwise. Since the time of the first simulations was known, it was important to keep the number of cells as low as possible, thus a structural grid was preferred. To get that in all regions of the kiln, a method of multizone with hexa mapped mesh and hexa dominant free mesh was applied in these regions.

### 3.1.2 Final geometry and mesh

Results from simulations later showed that the cubes were a poor approximation of the ceramics due to an unrealistic low temperature in the centre, that probably were caused by the long distance to the core. To change that, the cubes were replaced with 10 centimetres thick plates that stood vertically. To be able to produce the structural mesh, the firewall was reduced from the real 65 to 50 millimetres, to fit with the 5 centimetres mesh. To avoid backflow from swirls behind the ceramics, the ceramics were placed one metre above the inlet, and to avoid the cold outer walls and to enhance the flow through the ceramics, each ceramics part had at around 20 decimetres between both other ceramic parts and 40 to 55 centimetres to the outer walls. The kiln and ceramic geometry is seen in Figure 3, where the kiln bottom area was 2.8 times 2.8 metres, the heights in the corners was 3.15 metres, the total heights was 3.45 metres and the firewall was 2.5 metres tall.
Figure 3 Schematic figure of the dimensions of the kiln. The firewalls is 65mm and the thickness of the ceramics is 100 mm and the distance between them is 200 mm.

The parts of the kiln were also divided into smaller parts to enhance a production of a structural mesh. To add more cells to the plates, for the same reason as the wall of the pottery as mentioned above, local inflation were added to the ceramics with two layers and a growth rate of one. The number of cells in the ceramics were before the inflation around 250 000, and with the inflation 316 453. To evaluate the quality of the mesh aspect ratio and orthogonal quality was used, and the mesh had an aspect ratio of 16 and orthogonal quality of 0.4 and as seen in Figure 4 the mesh was fully structured except for the ceramics with the inflations.
3.1.3 Discarded simulation models and settings

For the evaporation the water were first divided into three groups, water sites needed for absorption, absorbed water that has been absorbed and water vapour. The mix of fluids was in the mixture template and the specific heat capacity was set by mixing law, viscosity by ideal gas mixing law, mass diffusivity by kinetic theory and the absorption coefficient by a UFD for the ceramics and the firewall. The water site was basically water liquid but without mole weight, specific heat capacity, standard state entropy and enthalpy and was included in the radiation. The absorbed water was just liquid water and water vapour was just water vapour except that the viscosity was determined by the laws of mixing.

The evaporation of water was first modelled with species transport and volumetric and wall surface reactions where the turbulence-chemistry interactions were laminar finite rate. Evaporation, desorption, and condensation, absorption, are too fast to be simulated in Fluent, therefore the pre-exponential factors for both of them are lower than in reality but only to the requirement that the equilibrium coefficient is correct. That means that the total reaction is the same because both the forward and the backward reaction is decrease equally. Both adsorption and desorption was a wall surface reaction but with no activation energy for absorption and 39 kJ/mole for desorption, which is approximately the enthalpy of evaporation (12). Both pre-exponential factors were assumed from reaction calculations where the temperature was assumed to increase independent of the reaction
during a certain amount of time. The calculation are from Nilenius, 2010 (1), and can be found in APPENDIX A. Both reactions use the same mechanism where one site was used with wall surface reaction and a site density of 25 moles/m² and an initially water coverage of 90%. The amount of water in the ceramics that was removed during the process was about 20% that is represented by the site density, which is a reasonable amount calculated from real measurements from Kalali, 2010 (3), and Schotte, 2010 (2).

3.1.4 Final simulation models and settings

The turbulence model that was used was the RNG-ke model, because compared to the first used SST-model (1), it does not require that fine mesh near the walls but still can handle the low Reynolds number zone that will exist in this kind of operation. The energy equation was necessary to be able to simulate the energy. Radiation for the firewall, the ceramics and the outer walls was modelled with discrete ordinates with one iteration per radiation iteration, the absorption coefficient was set with and user defined function to 100 kW/(m²K), which came from Nilenius, 2011 (1), for the firewall and the ceramics and also the gas inside these volumes. The absorption coefficient was set that high so the outer surface would absorb most of the radiation and not get deeper into the ceramics or the firewall.

The ceramics were modelled as gypsum with its properties but the absorption coefficient for the radiation was set by the UFD. It was set as a porous material with a porosity of 0.1 and with a fixed value of zero for the velocity in all three directions. All of these came from Nilenius, 2011 (1).

Due to imbalance of the energy, some process in the evaporation absorbed more energy that it was suppose to, the evaporation model was replace with an specific heat capacity increase for the ceramics between 50 and 150°C that correspond to the amount of energy needed to evaporate all the water in the ceramics. Unfortunately, there were some errors in the calculations and the extra specific heat capacity only represents a water content of 16%. This was done to an own copy of the gypsum, so the outer walls and firewall that also uses gypsum as material is not affected.

The outlets design was unknown prior the building of the kiln, thus it was modelled as a pressure outlet. That will both give the opportunity to start without the exact design, but it also simplifies the adaption of the model to other kilns with different designs. The backflow temperature was changed by hand, as the temperature in the outflow increased.

To be able to evaporate enough water in the ceramics and heat it, the flow of the inlet has to be approximated and it was assumed constant during the simulations. The amount was calculated from how much air, cooled 800°C, was needed to evaporate the water in eight hours and heat the ceramics to 800°C. To that, an assumed efficiency of 50% is added and the full calculation can be seen in appendix B.

The outer walls thermal settings was modelled as a mix of convective and radiation. The heat loss from outer walls is modelled in the software as convective with walls of 18 centimetres, outside air of 30°C and a heat coefficient of 25 W/(m²K), which is an average value for free convection in air according to Welty et al, 2001 (13). The radiation was activated by setting the internal emissivity to one and internal emissivity to zero.

The solution methods where all from Nilenius, 2011 (1), where the used pressure-velocity coupling scheme is SIMPLEC, the gradient was solved with least squares cell based, the pressure with standard.
The momentum, turbulent kinetic energy, energy and discrete ordinates were all solved with second order upwind and at last the turbulent dissipation rate were solved with first order upwind. In the solution control the under relaxation factors were all default values.

There are three parts in this simulation process. First, there is the part where flow was stabilized and in this simulation, that was done by cancelling everything except the flow and make the calculations steady state. That gave a solution with a velocity profile that was used to initialize the next part, where the temperature and energy flow was stabilized and was calculated for 100 seconds with one-second time steps. In the last step, the heating of the ceramics and the modelled evaporation of the water and this was done with ten seconds time step for seven hours.

3.2 Measurements and Validation

CFD-simulations at these scales are always results from models of the reality, thus the results has to be confirmed to be close enough to the reality. The two most important parameters in this case are the temperature and the flow of flue gases. Unfortunately the kiln that this was supposed to be measured in were not built during the project and this section only contain how it was supposed to been accomplished.

The temperature is a crucial parameter for the quality of the pottery, both to an absolute value and the speed of the temperature increase. The pottery temperature has to reach at least 900°C to be sintered and not only dried to achieve the best quality. The increase of temperature shall also not be too fast, since then the pottery will crack. A stainless steel probe that measures the temperature over a certain length of the probe was supposed to measure the temperature. Due to the contribution of radiation to the measurement the probe should have been covered by a tube of stainless steel and were supposed to be as blank and has as low emission coefficient as possible, the so only the wanted convection was affecting. To allow the convection it would have been important to keep the protection some distance from the probe, thus, the tube would have been a good alternative. The temperature should have been measured both at the inlet to the chamber to confirm the boundary condition of the inlet, and at various places in the chamber, for the temperature distribution to be evaluated and the simulation to be validated.

The volumetric flow of the inlet determines the speed of the flow and the amount of heat that is transported into the chamber. The speed is crucial to the temperature distribution along with the physical design of the kiln, and the amount of heat is important to the temperature of the pottery. The flow was supposed be measured at the inlet with a Pitot tube in order to determine this.

Since the new kiln will use coconut shell briquettes as fuel, this change was wanted to be evaluated and this was supposed be done by asking the users of the kiln. The temperature in the fireplace would have been measured. There were also thoughts about letting the carbon dioxide to be measured so the excess of air to the combustion could have been determined.

The weight of the ceramics should have been measured before and after the firing, so both the amount of evaporated water and weight of the dry ceramics can be determined. The amount of water would have been easily compared with the simulations, and the amount of ceramics would have been important to compare with the simulation so the amount is equal.
4 Results
First, there will be results from a simulation were the adsorption of radiation to the ceramics was neglected, and then one where it was not. Then the results from the period in Indonesia will be presented and at last the visit in Höganäs.

4.1 CFD Results
The other big difference between these two simulation except the radiation, were that in the first simulation the energy flow stabilization part were 500 seconds one second time steps and that the time step after that were 30 seconds.

4.1.1 Simulation without radiation
After 28700 seconds, which is about 8 hours, the lowest temperature of the ceramics was 378K, the highest 1012K and the average 760K. The temperature at the diagonal views in Figure 5, in the inlet and the opposite corner there is hotter that other places in the kiln. There are also very cold spots in the ceramics, the air around the ceramics is rather cold and there is space above the ceramics that is cold. The space below the ceramics is around 960K, which was the backflow temperature of the outlet, since a large part of the outlet had backflow.

Figure 5 Contours of temperature at the diagonal, no radiation
Unfortunately there was not only cold in the ceramics, also the outer surface of the ceramics was cold with the coldest temperature at 522K, see Figure 6. It is also visible that the highest outer temperature of the ceramics are 1020K and that is located in the opposite corner of the inlet.

Figure 6 Contours of temperature at the surface of the ceramics, no radiation

The uneven temperature distribution in the ceramics predicts from the temperature distribution above the ceramics, where in Figure 7 the temperature right above the ceramics is to the left and 0.5 metres above is to the left. Note that the temperature scale is different for the two surfaces.
Figure 7: Contours of temperature just above the ceramics to the right and 0.5m above the ceramics to the left, no radiation.

Figure 8 shows the velocity vectors, coloured by the temperature and it's clear that the strong inlet takes the energy and the flow up to the ceiling and it's spread uneven when it hits the ceiling, where the corner in the bottom of the right picture gets the least amount of heat. It is also visible that the strong movement of flue gases makes an swirl and leaves a colder area in the middle of the kiln.

Figure 8: Velocity vectors coloured by temperature in the whole kiln, no radiation.

The swirl is very clear in Figure 9, which shows only the negative Y velocity right above and below the ceramics and at the outlet, which is almost only in the opposite corner. It is also visible that a larger part of the flow goes to the left side rather than the top side of the kiln according to the figure. Here is also the big backflow from the outlet visible.
4.1.2 Final simulation with radiation

After 28 700 seconds, which is about eight hours, the average temperature in the ceramics is 677K, the minimum is 491K and the maximum is 897K. As seen in Figure 10, the hotter spots are again at the inlet and in the opposite corner, but this time the temperature in the corner is lower, so much lower that the temperature below the ceramics are in the same order of magnitude. The temperature below the ceramics is here also around the backflow temperature. It is also visible that the ceramics and the cold space above the ceramics have a significant lower temperature, but the cold space above have a similar shape that in the case with no radiation to the ceramics.
The temperature of the ceramics' surface are between 612K and 917K with a mean value of 768K, as seen in Figure 11 and it is also visible that the parts facing the outer walls and the opposite corner of the inlet that is the hottest. The lower parts of the ceramics is also hotter that the upper parts.
The uneven temperature distribution in the ceramics predicts again from the temperature distribution before the ceramics. In Figure 12 is the temperature at the very top of the ceramics is to the left and the temperature 0.5 metres above the ceramics is to the right and it is visible that a lot of the energy goes to the opposite corner, but also to the corner to the lower left. Note that the temperature scale is different for the two surfaces.
Figure 12 of temperature just above the ceramics to the left and 0.5m above the ceramics to the right.

Figure 13 shows the velocity vectors coloured by the temperature and it is clear that the flow goes to the opposite side of the inlet and little to the same side, as in the case with no radiation. The cold space in the middle created by the strong swirl in the kiln is also visible.

Figure 13 Velocity vectors coloured by temperature in the whole kiln.
The swirl becomes very clear in Figure 14 where the negative velocity, the velocity downwards, views in the outlet, below and above the ceramics. The resemblance with the case without radiation is large.

In Figure 15, the mean temperature in the ceramics is plotted over time, and it is visible that the increase is rather continuous, except during the last two to three hours where it slows down.
4.2 Sensitivity analysis of the simulations

The first steady state simulation iterated until the solver detected convergence with default tolerance values and in Figure 16 is the velocity profile at the diagonal for the converged solution and 145 iterations before. As seen, the velocity difference is small and the solution considers converged and is used in further simulation.

Figure 15 Plot of mean temperature in the ceramics over time

Figure 16 Contours of the velocity and its difference between steady state simulations at 6500 and 6645 iterations, 6500 iterations contour to the left, the difference to the right
The next is to evaluate the first time step period, where two simulations, one with one second time steps and one with 0.5 second time step, calculates for 100 seconds and compared. Figure 17 shows the velocity contours of 0.5 second to the left and the difference between the two cases to the right and the difference is very low. In Figure 18 is the temperature, again 0.5 seconds result to the left and the difference to the right, and it is very clear that the biggest difference is 50°C and is located in the backflow area, otherwise it is at the most 15°C.

![Figure 17 Contours of the velocity and its difference between 1 second time steps and 0.5 seconds at flow time 100 seconds, 0.5 seconds to the left, difference to the right](image)

![Figure 18 Contours of the temperature and its difference between 1 second time steps and 0.5 seconds at flow time 100 seconds, 0.5 seconds to the left, difference to the right](image)
In the last time step period the one second time step was continued from the first 100 to 300 seconds, and compared with the used ten seconds time step at the same flow time. The velocity that is seen in Figure 19, where the one second time step result is to the left and the difference to the right, the difference is again very low. Figure 20 show the temperature contours, with the one second time step result to the left and the difference to the right and here the difference is low, at the most 10°C except for some areas in the firewall.

Figure 19 Contours of the velocity and its difference between 10 second time steps and 1 seconds at flow time 300 seconds, 1 second to the left, difference to the right

Figure 20 Contours of the temperature and its difference between 10 second time steps and 1 seconds at flow time 300 seconds, 1 second to the left, difference to the right

Investigation of the number of radiation is showed in Figure 21 where the plot to the left is during the first 500 seconds, where the change from one to ten seconds time steps occurs after 100 seconds, the
The plot to the right is between 10,000 and 15,000. The first one you can see a slightly change in the gradient of the temperature increase at 100 seconds. In the second one there is an extra line that starts at 13,100 seconds, which is a test where the radiation iterations per iteration is increased from one to four with a try to decrease the computational time.

![Figure 21 Plots of the mean temperature in the ceramics in Kelvin over the time](image)

Since the temperature change in these simulations is either in the flow or in solid materials, the velocity considers as the most important variable for the mesh, therefore performs mesh adaption dependent of the velocity. To that, the high flow in the inlet, large time steps and large cells in the mesh makes the flow to pass several cells during one time step, which makes the velocity a more critical parameter to adapt the mesh. The refinement was done to 12,366 cells and increased the number of cells up to 403,015. As seen in Figure 22, where the velocity result from the adaption is to the left and the difference to the right, there are differences that are rather big in the inlet and at the ceiling where a lot of the adaption probably has occurred.

![Figure 22 Velocity contours after mesh adaption dependent of velocity, results after adaption to the left and the difference to the right](image)
4.3 Results from study period in Indonesia
Since the kiln never was constructed, there are no direct results, but there are still some things to illuminate.

The pottery from Yogyakarta exports all around the world and the potters are afraid of losing these markets if they keep firing with wood, so the will to change fuel is high.

The owner of one of the downdraft kilns told that they got temperatures up to 1000°C in that kiln, but how he knew that is not known. Anyhow, they at least know that the downdraft kiln reaches much higher temperatures.

The clay that they have been using in Kasongan, the village outside Yogyakarta where the kiln were supposed to be built, is about to finish, which implies that they have to use other clay. The closest place to get clay from have a different type of clay, which has to reach 900°C to achieve good properties and since that cannot be done with the updraft kiln, they really need to get downdraft kilns.

4.4 Results from Höganäs
In Höganäs they does not have any full scale production anymore, so the kilns that are left are just for display. Unfortunately there was not any potter there to explain the kiln, but the design of the kiln told a lot. As seen in Figure 23 the kiln is very large and the outer walls were almost 5 decimetres thick. But it is the shape of the walls that are interesting, it is almost shaped like a half sphere and at the top, there is a small hole. Every kiln had around eight fireplaces and an equal amount of inlets. The firewalls at each inlet is around two times five decimetres, and the height is between five and ten decimetres.
5 Discussion

5.1 Discussion of the simulations
The ceramics will look and be packed different for every batch, thus the ceramics cannot be correctly modelled and to approximate the ceramics with some model are almost necessary. Nevertheless, how they are modelled is more unsettled. First, the ceramics are often hollow with rather thin walls and since big kilns like this easily get too many cells, the model cannot be kept that way and they have to be larger than normal. That both create problem of how that is modelled the best way and it creates an error to the temperature due to the larger distance to the core and smaller outer surface for the ceramics, that both are important to the energy transfer. The smaller amount of surface area also affects the flow and the radiation, since the flow then meets a bigger flow resistance in reality and the radiation have fewer surfaces from where the radiation can emit and absorb. It might also be problems with the fact that the ceramics in reality is placed upon each other in the kiln and at the bottom of the kiln, which introduces the question of how the energy transfers is affected by the floating ceramics in the simulation in contrast to the stacked ceramics, but also how the outlet is affected.
The quality of the mesh is not the best according to the quality measurements, but since the mesh is fully structured except for the ceramic parts, the bad cells are probably there and thus, they have no flow and that decreases the error from the bad cells. According to the mesh sensitivity analysis, the mesh is of rather bad quality and should have been refined to achieve a more accurate result, but since the computational time is so long, this was not an option. It is visible that the largest change is right next to the wall in the inlet and the ceiling, which may be results of the poor wall treatment in too large cell in these spaces. Despite, the inaccuracy is probably low, since most of the difference is at the inlet and that will probably not affect the temperature and heat transfer to the ceramics, which is the most important in the simulations, and the mesh can be considered as good enough to be used to develop the Indonesian kilns.

The time step analysis is shown that the time steps are proper and in almost all the cases the difference is small or very small. The temperature mostly differs around one to two percents at the most and velocity difference is very low for all the cases except the steady state case, where the difference is 0.01 m/s in areas where the velocity is around zero, which still can be considered as low. The only exception is in Figure 18, where the temperature at 100 seconds differs 50°C at the most, this is in the backflow and is probably a result of an inconsequent raise of the backflow temperature between the both cases. More doubts are shown in the radiation sensitivity analysis, where a slight temperature gradient change is visible in Figure 21. The first thought was that it was because of that the time step itself was too high, but after that the test that is shown in the same figure, that changed. In the test, where the number of radiation iterations per iterations is decreased from one to four, the same lower gradient is displayed and thus, it is more reasonable to assume that it is the number of radiation iterations that cause the change at 100 seconds.

The water evaporation simulation was unsuccessful due to energy imbalance as mentioned, but that probably came from some errors from the radiation setup. The mixed settings for the outer walls with both convection and radiation were just done in the very last simulations and thus, there is a possibility that the error comes from the radiation and not the evaporation.

The specific heat capacity increase to evaporate the water was not only too low, the model implied also that there is no water there and the heating of the water is then negligible, which makes the model one step further from the reality.

The simulations clearly show that the velocity of the inlet flow is important for the temperature distribution and the inlet or inlet flow probably needs to be adapted for each kiln design and dimensions. The high inlet velocity creates a big swirl through the kiln that affects the results in two ways. First, the swirl push the flow with the energy to the opposite corner and side, which cause a big cold space in the middle where the ceramics are. The temperatures in the ceramics to the sides closest to the firewall probably have a higher temperature than the centre due to radiation. The swirl also creates a backflow in the outlet that make the results dependent of the backflow temperature and the manual change of the backflow temperature during the simulation is not optimal. If the flow is optimized to not create any swirl that error would probably be negligible.
The result shows similar patterns for the Y velocity and the temperature distribution in the flow, the higher Y velocity downwards, the higher temperature. In this case, the swirl probably affects this and makes it more coinciding, but it might still be possible without the swirl.

The overall result shows a low temperature, for both the surface and the whole ceramics where the mean temperature of the ceramics only reached 404°C and the minimum temperature of the outer surface was 339°C, which is lower than what is necessary for the vitrification process to start. The optimal would have been if even the centre of the ceramics is vitrificated, after that it is favourable if at least the surface of the ceramics is vitrificated. The reasons for this low temperature are many. First, the real temperature at inlet is unknown and it could be higher than assumed, since it is probably hard to get the ceramics up to a temperature 100°C below the inlet temperature. The real flow of the inlet is also not known, and a higher flow would increase the amount of energy into the system and thus, decrease the time to reach a certain temperature. To this problem the discussed thickness of the ceramics matters and must be taken into account for the comparison with reality. There is also visible in Figure 15 from the mean temperature in the ceramics over time that the change in specific heat capacity does not affect the mean temperature in the ceramics. Since the temperature increase is the same even if it requires more heat, it indicates that it cannot be the first energy step, the convection, that is rate determining and but it is probably the conduction, which adds even more disadvantage for the thicker models of ceramics.

The different simulations show that the radiation is affecting the result and it is clear that it produce a more even temperature distribution, probably because the warmer areas can radiate energy to colder area. However, the mean temperature in the ceramics is lower with the radiation, which is a little unexpected theoretically. Too few radiation iteration or too large time steps might cause this.

5.2 Discussion of the kilns design

With the assumption that the Swedish potters have made a good work with their kiln design, the following designs can assumes as good. The height of the firewall is probably of less importance and can retain low to reduce the building material. The spherical shape of the outer walls probably prevents the kiln to explode or crack. The hole at the top probably opens after firing to decrease the cooling time. The fact that the kiln has multiple inlets also strengthen that the flow of the inlet are important since then the potters can keep the firing at constant rates for every fireplace and change the heat flow into the kiln by closing and opening fireplaces, instead of changing the fire rate at one inlet. That also implies that the area of the inlet is important, since if the fireplaces are designed for a certain fire rate, the area of the inlet might need to match that volume flow to obtain an optimal speed for the flue gases. However, the multiple inlets might simplify that, since if the speed is higher than optimal and two opposite fireplaces are burning, the flue gases from both inlets will collide in the middle of the kiln and that might create an more even temperature distribution in the kiln, due to the turbulence it would create.

6 Conclusion

Real measurements were not accomplished in this project and thus, the simulations cannot be validated and inlet flow and inlet temperature had to be assumed. The inlet flow is assumed from the energy
requirement for evaporation and heating. There is a possibility that both the inlet flow and temperature are underestimated. The inlet flow is also, with the design of the kiln, important to achieve a proper inlet velocity that is crucial for the temperature distribution. Every kiln design probably has a velocity interval that is good, but if multiple inlets are used and the flow collides in the kiln, the velocity can probably be much higher.

Despite all approximations and assumptions and that it is uncertain how good the model predicts the reality, it probably would work as a development tool for the kiln design, since the errors would probably be the same for both designs.

6.1 Further development and work

The water evaporation should be good to implement in the model and it might give information of how the evaporation affects the process, i.e. an optimal packing distance might be determined. Nevertheless, the model for the shape of the ceramics has to be evaluated for this kind of simulations.

Validation of the simulation models is important, it can determine if any models are inaccurate which is crucial for the development. If the validation is successful, it proves the accuracy, which is good for the development and the model might be useful for simulation of other processes. With the validation there would also be good to continue the development since the temperature distribution might not be the best. Evaluation of multiple inlets and baffles is possible development areas.

Since the velocity profile and the temperature distribution correlate, the possibility to use the velocity profile to evaluate the temperature distribution exists. That would decrease the computational time to just a small fraction of this simulations, but it also implies that the measurements must be good enough to evaluate a temperature distribution and it has to be comparable with the simulations. It would also decrease the complexity of the simulation since the problem would not need any energy equations, no radiation, no water evaporation and no time dependency.
Reference list


12. ANSYS, Inc. ANSYS 13.0 Dokumentation. 2010.


Appendix A

The pre exponential calculations from Nilenius, 2010 (1):

clear all
close all
clc

global ka kd dH_vap q V_tank V_bodies n_h20 R T

V_tank=2*3*1.8+1^2*pi*3; %m^3 volume of tank
V_bodies=0.4^3*24; %m^3 volume of porous bodies
rho_bodies=2000; %kg/m^3
wt_h2o=0.2 ; %wt% of water in bodies, initially
m_bodies=V_bodies*rho_bodies %kg weight of porous bodies
MW_h2o=18; %kg/kmole mole weight of water
n_h2o=m_bodies*wt_h2o/(MW_h2o*1e-3) %mole h20 per m^3 porous body
R=8.31447e-3; %kJ/mole K gas constant
dH_vap=1.0*1404*1.5*MW_h2o*1e-3 %kJ/kg/kmole=kJ/mole approximated heat of vaporization for bounded water at 300 degree C (8)
dH_vap=40 %kJ/kg/kmole=kJ/mole approximated heat of vaporization for bounded water at 300 degree C DoD

q=0.18; %m^3/s
kd=50 ;
ka=60;
% tspan=[0 3600]
% tout=linspace(tspan(1),tspan(2))
[t y]=ode15s('hast',[0 1000],[0,0.9]);
% plot(t,y(:,2))
% hold on
figure(2)
plot(t,y(:,1))

function dydt=hast(t,y)

global ka kd dH_vap q V_tank V_bodies n_h20 R T

c=y(1);
theta=y(2);
T=200+273.15 +0.1*t %K
r_des=kd.*exp(-dH_vap./(R.*T))*theta
r_ads=ka*c*R*T*(1-0.9*theta)

dcdt=-q*c/V_tank+(r_des-r_ads).*V_bodies./V_tank

dydt(1)=dcdt;
dydt(2)=dthetadt;
dydt=dydt';
## Appendix B

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