# Numerical Modeling of Anode Baking Process with COMSOL® Multiphysics

P. Nakate[1,2], W. Voogd de[3], D.J.P. Lahaye[1], C. Vuik[1], M. Talice[4]

1. Department of applied mathematics, Delft University of technology, Netherlands

2. Aluminium and Chemie Rotterdam B. V., Netherlands

3. Faculty of science, Leiden University, Netherlands

4. pm2engineering, Cagliari, Italy

## Abstract

The anode baking process has gained significant attention since the 1980s due to its importance in Aluminium industry. A good anode baking process strives to achieve multiple goals including reduction of NOx from emissions. NOx generation is mainly due to the high-temperature distribution around the burner and the air/fuel ratio. Therefore, understanding of the physical phenomena around the burner is of importance. The mathematical model in this respect can provide significant information. The underlying problem of NOx optimization in anode baking furnace is characterized by the different physics such as the turbulent flow of air and fuel, combustion of fuel and volatile matter, heat generation due to combustion process, conjugate heat transfer through walls and radiation. The objective of this work is to systematically develop the mathematical model of the anode baking process by considering all the physical phenomena. As a first step, turbulent flow model is developed with Spalart-Allmaras and k-ε turbulence models. In the subsequent model, a single step methane combustion reaction with eddy dissipation combustion model. In this model the effect of radiation is also checked by implementing P1 approximation model. The validation of results of turbulent flow model obtained by COMSOL® Multiphysics is carried out by comparing with other simulation environment, namely, IB-Raptor code. The results of reactive flow model are still in progress. However, preliminary analysis provides reasonable agreement with expected finding. The effect of radiation is also observed by varying absorption coefficient of the participating medium. The model developed in this work is based on assuming boundary conditions that lower the nonlinearity of equations. However, in order to compare results with actual furnace conditions, tools that can resolve highly non-linear equations would be needed.

## Introduction

Anodes are important in Aluminium industries as it accounts for 15% of the costs [1]. The anodes are mainly used in the extraction process of aluminium from bauxite in the Hall-Hèroult process. The raw anodes usually referred to as green anodes have 85% of pitch and 15% of volatile matter [2]. In order to be efficient in the Hall-Hèroult process, these anodes should have high mechanical strength, low reactivity in the process and should be highly conductive. In order to gain these properties, green anodes need to be baked. Therefore, the anode baking process has gained significant attention since 1980's [2]. The anode baking process consists of multiple physical phenomena such as turbulent flow, combustion process, conjugate heat transfer, and radiation. The process is highly energy intensive as well as releases environmentally hazardous gases such as $CO_2$ and $NO_x$. Therefore, an ideal anode baking process strives to achieve multiple goals such as reducing energy utilization, reduction in NOx, soot-free combustion and improving quality of anodes. This can be achieved by optimization of the process by mathematically modelling the interdependence of multiple physical phenomena.

The mathematical modelling of the anode baking process has been developed and improved significantly in past years. The first attempt of mathematical simulation of horizontal flue ring furnace was performed by Bui et. al. in 1983 in which they treated furnace as counter-flow heat exchanger [3]. These early developed models form the basis of the models that are developed at the later stage. More recently, an advanced 3D transient model has been developed by Severo et. al. which can be used for optimization of flue design and furnace optimization [4]. Severo and Gusberti also developed a user-friendly software for the simulation of anode baking furnaces [1]. However, the optimization of burner design to study the NOx formations is not very clear. Oumarou et.al. in his recent work developed a dynamic process model of

anode baking furnace to investigate the effect of temperature variation in vertical component by considering a vertical component of flue gas [2], [5], [6]. However, the model is not able to provide the combine optimal of saving energy, reducing emissions and maintaining good anode quality. Meanwhile, Tajik et. al. developed a model using Ansys Fluent in which effect of flue wall design on the flow field, combustion and temperature has been presented [7], [8]. The finite volume method is used in Ansys Fluent. Whereas, COMSOL® is based on the finite element method. It would be interesting to compare the results with two approaches. A compelling study have been performed by Grègoire and Gosselin, in which three combustion models have been compared for simulating anode baking furnace in Ansys Fluent [9]. However, the model that seems promising needs calibration which can be tricky. Therefore, a significant development has been done in the modelling of the anode baking process. However, the modelling that focuses on reducing NOx is still obscure.

The main aim of the present work is to develop a model that focuses on reducing NOx emissions. COMSOL® Multiphysics has been chosen for its capability of handling multiple physical phenomena. In the present paper, the turbulent flow model is developed as a first step. The results are validated by comparing with another simulation environment, i.e. IB-Raptor code developed by pm2engineering from Italy. The model is then extended by adding a single step combustion reaction of $CH_4$. Radiation being the important mode of transfer of heat in the process, is also added in the subsequent step. The results of the reactive flow model with radiation are not yet validated. However, they provide results that align with expected findings. Currently, an attempt to extend this model to 3D geometry is in process.

## Model Equations

Anode baking process is characterized by multiple physical phenomena which can be translated into mathematical equations. However, in order to solve these equations, certain assumptions are needed that simplify these equations. These simplified equations form the basis of the numerical model. In this paper two models are described, wherein, the second model is the continuation of the first model. The first model describes the non-reactive turbulent flow of air and fuel (methane) which is validated by comparing with another simulation environment. Whereas, the second model outlines the single step reaction of methane and air, along with their mixing by the turbulent flow. The heat generated by the combustion process is accounted on the basis of the extent of reaction and heat of reaction. The model also defines the surface to surface transfer of heat through radiation. In this section, the established simplified models that are used in the present work are described.

### Reynolds-averaged Navier-Stokes equation (RANS)

The flow of air and fuel in the anode baking process undergo significant fluctuations due to the presence of baffles and tie-bricks that are needed for the structural stability of the flue wall. Moreover, the high efficiency of the mixing of fuel and air is desired for effective combustion. The flow conditions in the flue wall, therefore, are such that the flow is highly turbulent. Modelling turbulence is complex in its original form due to the complicated mathematical expressions. RANS equation, in this respect, can be of importance as it simplifies the equation by taking the time average of Navier-Stokes equation providing the mean flow equation. Here, the turbulence is classified into two components, namely, mean part and fluctuations. The quantity that defines these fluctuations in RANS equation is referred to as Reynolds stress. This term is related to the rate of deformation and is defined in terms of turbulent viscosity and average kinetic energy by Boussinesq. The Number of models are available that relate turbulent viscosity and average kinetic energy. In the present paper, two such turbulence models, namely, k-ε and Spalart-Allmaras model are studied. The k-ε turbulence model consists of two scalar transport equations, one for turbulent kinetic energy and another for turbulent energy dissipation rate. The Spalart-Allmaras model, whereas, solves for only one variable, i.e. undamped turbulent viscosity parameter. Apart from the number of variables that are solved, these turbulence models also differ in the way the flow is resolved near walls. The Spalart-Allmaras model being a low-Reynolds number model, resolves the flow till the wall, whereas, the k-ε model uses wall functions to approximate flow near walls. This comparison is important in this research, as both turbulence models have relevance with respect to different goals of ideal anode baking process.

### Eddy dissipation model

In the anode baking process, the air and fuel enter the furnace from the different inlets as well as at different time. Therefore, the combustion of fuel can be regarded as non-premixed. Different models are available that relates the rate of reaction in the turbulent flow. The rate can be either assumed to be

controlled by turbulent mixing or reaction time. The eddy dissipation model is the simplest form that defines the rate of reaction in terms of turbulent mixing. In this model, the reaction is assumed to occur at the infinitely fast rate. Therefore, turbulent mixing is the significant timescale for the rate of reaction. The reactive turbulent flow model in the present paper assumes the single step reaction of methane and the rate of reaction is governed by the eddy dissipation model.

### P1 approximation model

Radiation is another important physical phenomena in the anode baking process due to the high temperature in the furnace. The effect of transfer of heat by radiation is expected to be significant in the model. P1 approximation model is one of the simplest models to calculate the total radiation intensity term from the radiative transfer equation. The radiation intensity is assumed to be isotropic in this model. This simplifies the model and reduces the computational costs.

These three well-established models form the basis of the numerical models that are developed so far in the present work. The detailed explanation of these models can be found in the report [10].

## Simulation details

The anode baking process consists of multiple physical phenomena that are dependent on each other. COMSOL® Multiphysics being a powerful tool for integrating multiple physics is used for numerically modelling the anode baking furnace. A 2D section from a heating zone is chosen as the geometry for both turbulent flow model and the continuation to reactive turbulent flow model with radiation. Figure 1 shows this geometry along with the inlet and outlet for air and fuel.

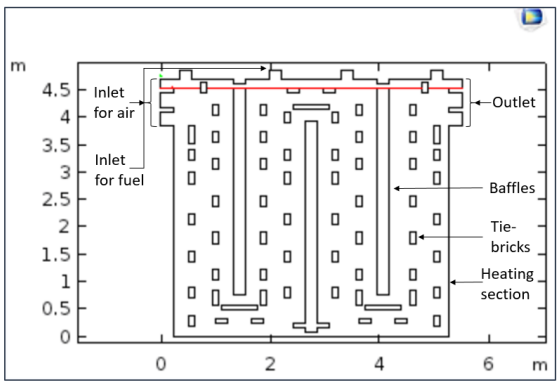



**Figure 1.** Geometry along with the boundaries for two models in COMSOL® Multiphysics

For modelling the turbulent flow with k-ε turbulence model, 'Turbulent Flow, k-ε' physics interface and, for Spalart-Allmaras model, 'Turbulent Flow, Spalart-Allmaras' physics interface from the CFD module is chosen. The density of the air is modified according to the equation of state and is a function of pressure and temperature. The change in density of air due to mixing with fuel is not accounted for, in this model. Both turbulence models require user controlled boundary layer meshing so as to have desired wall resolution [11]. The splitting function is used to modify meshing near corners. The convergence behavior of simulations, especially in the case of the Spalart-Allmaras model, is highly affected by the elements at the boundaries and corners, due to high gradients at these points. In these models, the boundary conditions are adjusted such that the non-linearity of the model is decreased. The initial and boundary conditions for k-ε and Spalart-Allmaras model are as shown in the following Table 1**.** These boundary conditions are motivated by the model developed in another simulation environment (IB Raptor code) that is used for validation.

**Table 1.** Initial and Boundary conditions for turbulent flow model

| **Initial conditions** | **k-ε** | **SA** |
|---|---|---|
| Velocity | 0 | Solution from k-eps model |
| | k and ε | Undamped turbulent viscosity parameter |
| Turbulence | 7.07E-07 $m^2/s^2$ and 1.10E-10 $m^2/s^3$ | 7.437E-04 $m^2/s$ |
| **Boundary conditions** | | |
| Air velocity at inlet 1 | 1.3 m/s | 1.3 m/s |
| Fuel velocity at inlet 2 | 5 m/s | 5 m/s |
| | k and ε | Undamped turbulent viscosity parameter |
| Turbulence at inlet 1 | 0.006 $m^2/s^2$ and 0.008 $m^2/s^3$ | 7.437E-04 $m^2/s$ |
| Turbulence at inlet 2 | 0.094 $m^2/s^2$ and 0.471 $m^2/s^3$ | 7.437E-04 $m^2/s$ |

The steady state conditions are implemented by using stationary solver. The default segregated solver with velocity and pressure as step 1 and

turbulent variables as step 2 is kept unchanged with MUMPS direct solver, with the default setting for both steps. The solver needs modification for initial CFL number. The mesh near boundaries is refined to such an extent that with higher CFL number, large oscillations are observed in the convergence plot resulting in the high residuals. Therefore, initial CFL number is set at 0.1. For the Spalart-Allmaras model, the default damping factor of 0.35 for step 2, that solves turbulence variable, is changed to 0.2 to achieve convergence. The change in the damping factor is not needed for the k-ε model.

The sequential model includes a single step reaction of methane and oxygen from the air. The 'Transport of Concentrated Species' physics interface from Chemical species transport module is used for modelling the combustion reaction. Five chemical species, namely, $CH_4$, $O_2$, $CO_2$, $H_2O$, and $N_2$ are considered in the model, $N_2$ being the chemical species used for a mass constraint. The density is governed by the ideal gas law with the temperature of 800 K as the model input. The flow is solved as described in the previous k-ε turbulent flow model and therefore, the convection velocity is based on the velocity field of the turbulent flow. The eddy dissipation model with an infinitely high forward rate constant and zero reverse rate constant is used so as the rate is defined by the turbulent mixing timescale. The reaction domain is assumed to be the complete 2D domain of the model. The initial and boundary conditions for reactive flow are defined as shown in Table 2.

**Table 2.** Initial and Boundary conditions for mass fraction of chemical species in reactive flow model

| **Initial conditions** | **$O_2$** | **$CH_4$** | **$CO_2$** | **$H_2O$** |
|---|---|---|---|---|
| Mass fraction | 0.21 | 0 | 0 | 0 |
| **Boundary conditions** | | | | |
| Mass fraction at Inflow 1 | 0.21 | 1E-05 | 1E-05 | 1E-05 |
| Mass fraction at inflow 2 | 1E-05 | 0.99 | 1E-05 | 1E-05 |

The 'Heat Transfer in Fluids' physics interface from Heat Transfer module is used for modelling the heat generated during the combustion process and transfer through radiation. Heat capacity at constant pressure for the mixture is defined based on the fraction of chemical species and heat capacity of the species at a particular temperature. Interpolation functions are used to obtain heat capacity at different temperatures for different species. Heat generated by the reaction is defined on the basis of the extent of reaction and heat of reaction as implemented in 'Round jet burner' tutorial by COMSOL. Radiation in participating media is used to model heat transfer through radiation. The model is run for three values of absorption coefficient using parametric sweep to check its effect. The emissivity is assumed to be 0.6. The initial and boundary conditions for heat transfer are defined as shown in Table 3.

**Table 3.** Initial and Boundary conditions for temperature and radiation variables in reactive flow model

| | **Temperature (K)** | **Emissivity** |
|---|---|---|
| **Initial conditions** | 293 | 1 |
| **Boundary conditions** | | |
| Inflow 1 | 800 | 1 |
| Inflow 2 | 800 | 1 |
| Outflow | | 1 |

The sequential model is also solved for steady-state conditions using stationary solver. The default segregated solver is implemented in which step 1 is for solving velocity and pressure, step 2 is for turbulence variables, step 3 is for mass fractions of chemical species and step 4 is for temperature and radiation variables. All steps use MUMPS direct solver with default settings. As in the previous model, damping factors and initial CFL number are modified.

## Results and discussion

In this section, the results that are obtained by non-reactive turbulent flow model and reactive turbulent flow model with radiation are presented. It is observed that the numerical convergence of both models is strongly dependent on the mesh, especially the mesh near boundaries. All results are obtained by COMSOL® Multiphysics version 5.3.

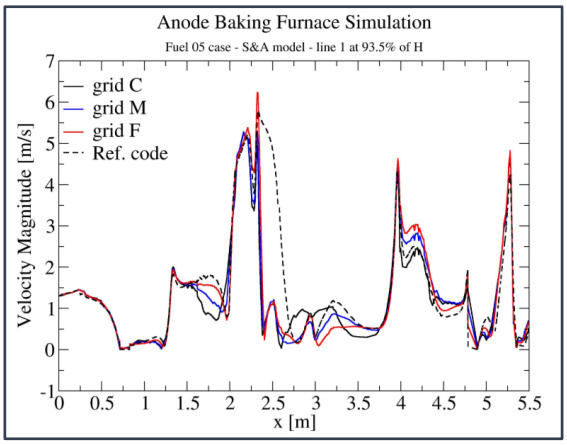
### Non-reactive turbulent flow model

The comparison of Spalart-Allmaras model and the k-ε model is the main highlight of the non-reactive turbulence flow model which is presented in the previous paper [11]. As mentioned earlier, this comparison is of importance as both models have their own advantages in the modelling of anode baking process. In the COMSOL® Multiphysics, wall functions are used as a boundary condition for walls in k-ε model, whereas, the Spalart-Allmaras model does not take that approximation and

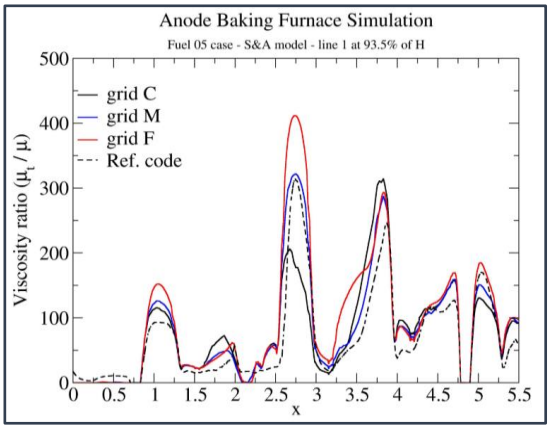
completely resolves the flow field near walls. In this section, the results of the flow field generated by the Spalart-Allmaras model are presented.

To validate the non-reactive flow model, the results are compared with different simulation environments, IB-Raptor code developed by pm2engineering from Italy. The model of IB Raptor code uses Spalart-Allmaras model. In order to have a concrete comparison, a horizontal line at 93.5% height from the bottom is chosen. This line gives an overview of all important areas of the furnace as shown in Figure 1.

Figure 2 shows the comparison of velocity magnitude and viscosity ratio results of IB Raptor code and COMSOL® Multiphysics Spalart-Allmaras model. It can be observed from Figure 2 (a) that the velocity magnitude generated by the two different codes are similar to each other. In both figures, Ref. code are the values generated by COMSOL. The slight differences which might be due to the mesh, type of solver and the approach of two codes are not significant. Similarly, Figure 2 (b) shows a plot for the viscosity ratio which also shows a good comparison between the two codes. The validation with IB Raptor code provides remarkable validation for the flow field and to proceed to the reactive flow model.




(a)



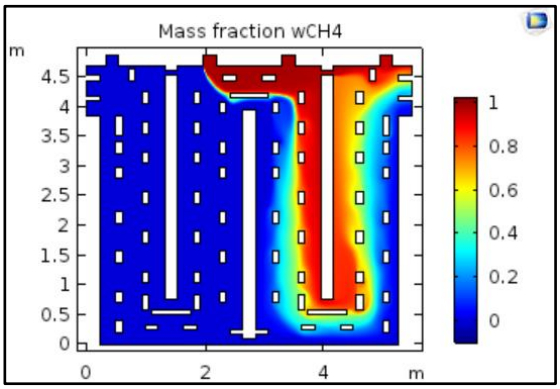

(b)

**Figure 2.** (a) Comparison of velocity magnitude (b) Comparison of viscosity ratio of models generated by COMSOL® Multiphysics and IB-Raptor code on line shown in Figure 1

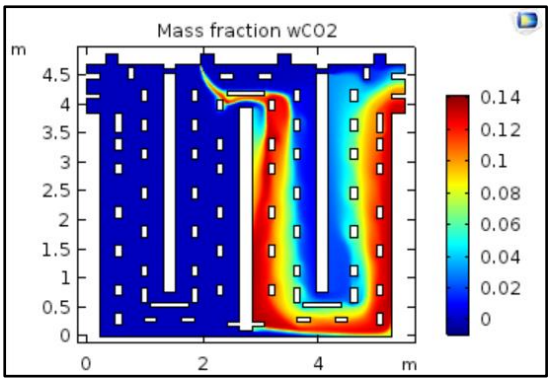
**Reactive turbulent flow model with radiation**

The turbulent flow model is extended by adding reactions, heat generation by combustion and transfer of heat by radiation. In this section, the results of this reactive flow model are presented.

Figure 3 (a) and (b) shows the mass fractions of $CH_4$ and $CO_2$ of reactive flow model. In the present model, the oxygen-methane ratio is much smaller than reality. Therefore, as can be observed from the Figure 3 (a), methane has some fraction near the outlet as the domain does not have enough $O_2$ to completely convert $CH_4$ into $CO_2$. Also, the reaction occurs as soon as $O_2$ mixes with $CH_4$ near the fuel inlet. Figure 3 (b) presents the mass fraction of $CO_2$ and the mixing interface of $CH_4$ and $O_2$. The generation of $CO_2$ is mainly in the interface where $CH_4$ mixes with $O_2$ which confirms that the reaction rate is governed by mixing timescale. This is the expected result from the eddy dissipation model which is captured by COMSOL® Multiphysics.




(a)




(b)

**Figure 3.** (a) Surface plot of mass fraction of $CH_4$ (b) Surface plot of mass fraction of $CO_2$ from reactive flow model

In this reactive model, the heat is generated by the combustion reaction of $CH_4$ and $O_2$. As the temperature in the domain is higher than 1000 K, the transfer of heat by radiation is significant which is accounted by P1 approximation model. The chemical species such as $CO_2$ and $H_2O$ are known to absorb notable radiation and therefore, radiation in participating media is used. Figure 4 shows the temperature distribution in the domain after considering heat generation and heat transfer by radiation. It can be observed that the increment in temperature occurs in the reaction interface which is also seen in Figure 3 (b). To analyse the effect of the radiation absorption coefficient, the temperatures at the horizontal line (from Figure 1) are compared in Figure 5. The comparison shows that before the reaction interface, the temperature for lower absorption coefficient is higher as compared to the temperature of higher absorption coefficient. Whereas, this trend is reversed after the reaction interface. This difference can be explained based on the increased temperature in the domain after the reaction interface. The exact explanation can only be established based on the future further analysis. However, this primary analysis shows that the effect of P1 approximation model can be analysed using COMSOL® Multiphysics.

## Conclusions

In the present work, COMSOL® Multiphysics has been used for modelling of a heating section of anode baking process. The process consists of multiple physical phenomena that are dependent on each other. Initially, a turbulent flow model is developed and validated by comparing results with another modelling code. This provides a validated flow field by CFD module of COMSOL® Multiphysics.

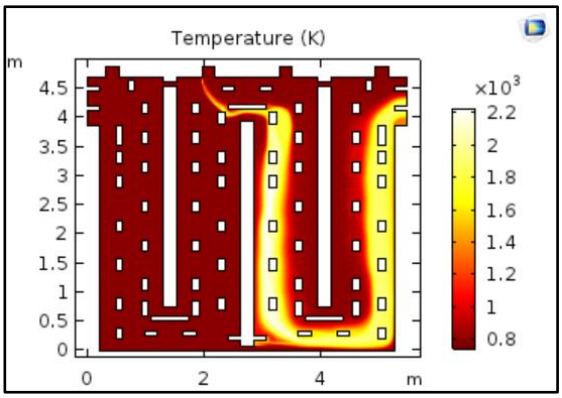



**Figure 4.** Surface plot of temperature in reactive flow model with radiation

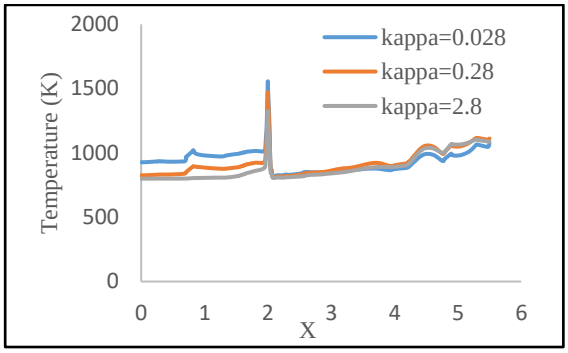



**Figure 5.** Comparison of temperature with different absorption coefficients of medium on line from the Figure 1

The subsequent reactive flow model with radiation provides reasonable results with chemical reaction and heat transfer modules of COMSOL® Multiphysics, though the validation is yet to be carried out. However, the modelling of combustion in COMSOL® Multiphysics is constrained by the basic eddy dissipation model. Detailed combustion models such as based on the probability density function would be needed for pollutant related studies.

## Further work

The extension from 2D to 3D modelling of a section of anode baking furnace is in process. Combustion modelling being important for NOx reduction study would be focused in more detail. Radiation is another leading physical phenomena in the process. More detailed radiation models such as discrete ordinate methods would be implemented as a next step.

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