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Nakate, Prajakta; Lahaye, Domenico; Vuik, Cornelis; Talice, Marco

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SYSTEMATIC DEVELOPMENT AND MESH SENSITIVITY ANALYSIS OF A MATHEMATICAL MODEL FOR AN ANODE BAKING FURNACE

Prajakta Nakate
Delft university of technology
Applied mathematics department
Delft, Netherlands
Email: P.A.Nakate@tudelft.nl

Domenico Lahaye
Assistant professor
Delft university of technology
Applied mathematics department
Delft, Netherlands
Email: D.J.P.Lahaye@tudelft.nl

Cornelis Vuik
Professor
Delft university of technology
Applied mathematics department
Delft, Netherlands
Email: c.vuik@tudelft.nl

Marco Talice
Co-founder
pm2engineering
Caglairi, Italy
Email: m.talice@pm2engineering.com

ABSTRACT

The anode baking process is developed and improved since the 1980s due to its importance in Aluminium industry. The process is characterized by multiple physical phenomena including turbulent flow, combustion process, conjugate heat transfer, and radiation. In order to obtain an efficient process with regards to quality of anodes, soot-free combustion, reduction of NOx and minimization of energy, a mathematical model can be developed. A mathematical model describes the physical phenomena and provides a deeper understanding of the process.

Turbulent flow is one of the important physical phenomena in an anode baking process. In the present work, isothermal turbulent flow is studied in detail with respect to two turbulence models in COMSOL Multiphysics software. The difference between wall boundary conditions for these models and their sensitivity towards the boundary layer mesh is investigated. A dimensionless distance in viscous scale units is used as a parameter for comparison of models with and without a boundary layer mesh. The investigation suggests that the boundary layer mesh for both turbulence models increase the accuracy of flow field near walls. Moreover, it is observed that along with the accuracy, the numerical convergence of Spalart-Allmaras turbulence model in COMSOL Multiphysics is highly sensitive to the boundary layer mesh. Therefore, development of converged Spalart-Allmaras model for the complete geometry is difficult due to the necessity of refined mesh. Whereas, the numerical convergence of k-ε model in COMSOL Multiphysics is less sensitive to the dimensionless viscous scale unit distance. A converged solution of the complete geometry k-ε model is feasible to obtain even with less refined mesh at the boundary. However, a comparison of a developed solution of k-ε model with another simulation environment indicates differences which enhance the requirement of having converged Spalart-Allmaras model for complete geometry.

1 Introduction

Anode baking process is the most important process in the aluminium industry. Presence of multiple physical phenomena such as turbulent flow, combustion process, conjugate heat transfer, and radiation makes this process complex to understand. Anodes are baked to achieve required properties for which a more uniform temperature distribution is desired inside the anodes while baking. Apart from this, a good anode baking process strives to achieve multiple goals such as uniform quality, soot-free combustion, lowest possible NOx generation, reducing maintenance cost and high furnace lifetime. The current practices fail to meet these goals to a complete extent. Therefore, a research study is required in order to understand the physics occurring in the process so as to meet these goals by improving or making necessary changes. Mathematical modeling in this respect can be of importance since it defines the system based on the physical theories and helps in predicting the behaviour of

different parameters with strong evidence of physics [1].

Several mathematical models of the anode baking process have been developed and subsequently improved since the 1980s. Transient 3D Model developed by Severo et. al. [2] accounts for all physical phenomena occurring in the process along with considering burner configurations. However, the number of chemical species as well as the complexity of chemistry considered in the model are limited. Therefore, prediction of emissions with this model is difficult. Moreover, the applicability of this model is limited for higher fuel velocity. Recently, a transient two-dimensional dynamic process model developed by Oumarou et. al. [3] investigates the effect of a vertical component of flue gas and thereby facilitates prediction of temperature variation in vertical direction. This model provides insights on the relation between anode height and maximum anode temperature. Also, low computational load and time are needed for simulating all sections of a fire cycle. But finding optimal for saving energy, reducing emissions and getting anode quality with this model is not possible. Therefore, a more robust model coupling all physical phenomena to account for multiple problems is required.

A good mathematical modeling practice suggests a structural development of the model by first implementing single physical phenomenon and thereby including consecutive physics. Moreover, validation of such structurally developed model at each stage is important to avoid issues at future steps. In the present work, this strategy of constructing step by step model has been implemented.

It is observed that obtaining a uniform flow field is the main challenge in anode baking process. Tajik et.al. [4] studied the effect of flue-wall design on flow field and observed that modification in the flue wall design significantly affects the flow field. Considering the importance of the flow field on the following involved physics, isothermal turbulent flow is chosen as the first step in the development of the model. Therefore, the focus of this paper is only on the turbulent flow in the furnace. Reynolds averaged Navier-Stokes equation is used to model turbulence. A model with the actual geometry is simulated using a k-ε model for defining Reynolds stresses. It is necessary to validate this model with other simulation environments to a large precision. In most CFD codes that deal with isothermal flows consider wall flow interaction as an important factor. Therefore, low Reynolds number flow model such as Spalart-Allmaras model is implemented in these CFD codes to define Reynolds stresses. In order to have a valid comparison with other CFD codes, the Spalart-Allmaras model is investigated in the present work as well. The striking difference between k-ε model and Spalart-Allmaras model is the way they resolve flow near the walls. This leads to modify numerical analysis near the walls.

The aim of this paper is to identify parameters that influence the numerical convergence of both models. In order to proceed this investigation, a bottom-up approach is implemented. A simple rectangular channel is modeled and later complexities are added in two steps to arrive at the actual complex geometry. A non-dimensional distance which represents a distance from the wall as measured from the viscous scale is used to associate the influence of the grid size near the walls on the numerical convergence. The study confirms the necessity of having finer mesh near the walls for the Spalart-Allmaras model. Whereas, the k-ε model uses wall functions thereby approximating flow field near the walls. Therefore, a relatively coarser mesh can be used for this model.

This study forms the basis of development of the model with multiple physical phenomena. Problems related to numerical convergence can be tackled by such a bottom-up approach. Moreover, flow field which is important physics in the overall model is resolved to a higher extent with this work.

2 Important concepts of model equations

Mathematical modeling of an anode baking furnace requires the understanding of multiple physical phenomena. The physics behind these phenomena can be complicated and may demand simplification while translating into a model. This is also necessary to have reasonable computational costs. However, these simplifications should be such that they retain the resemblance with the physical phenomena occurring in the actual application. Therefore, these physical phenomena are translated into mathematical equations which are further simplified using mathematical models that closely describe those mathematical equations [1]. In the present section, such model equations that are used to gain more understanding of the mathematical model of anode baking process, are described.

Fluid flow is of prime importance in an anode baking process. Typical Reynolds numbers of these flows imply that the flow in the furnace is highly turbulent. Other major phenomena that are part of anode baking process are combustion and heat transfer. However, this paper focuses on obtaining more knowledge of flow occurring in this process. Turbulence is attributed to flow and therefore can be described by the momentum equation. Mass conservation equation and momentum equation are two major balance equations that are solved in the present work. The physical models that are used in the present work are described in the following subsection.

2.1 Reynolds-averaged Navier-Stokes equation (RANS)

Turbulence is the most complicated physical phenomena in anode baking process, as it deals with a large number of fluctuations. Solving mathematical expressions that deal with these fluctuations might be complex. Moreover, in most of the industrial processes, time-averaged properties can provide significant desired information. Therefore, in this respect, RANS equation can be of importance. In this equation, spatial variations in phys-

ical properties such as density, viscosity etc. are averaged using the Favre average statistical approach. Turbulence can be simplified by decomposing velocity into the mean part and fluctuating part. RANS, as the name suggests, takes the time average of Navier-Stokes equation resulting in the mean flow equation.

RANS equation contains a nonlinear term which quantifies velocity fluctuations and is referred as "Reynolds stress". Reynolds stress increases as the mean rate of deformation increase [5]. Boussinesq proposed an equation, which relates Reynolds stress with the mean rate of deformation. Several models are available to define turbulent viscosity and average kinetic energy. These models differ in the way they solve flow field near walls and number of variables used to define turbulent viscosity. In the present work, the Spalart-Allmaras and the k-ε models are compared to elaborate their performance with respect to accuracy and numerical convergence.

2.1.1 Spalart-Allmaras model The Spalart-Allmaras model adds a single variable, undamped turbulent kinematic viscosity, to the set of equations. This model is a low Reynolds number model which implies that it can resolve flow fields completely even in the boundary layers. The turbulent boundary layer is comprised of three layers namely the viscous sublayer, the buffer layer, and the log-law region. Generally, the viscous sublayer and buffer layer are thinner by 2 order of magnitude as compared to the log-law region. The velocity profile in the viscous sublayer is directly proportional to the distance from the wall whereas, in the log-law region, the average velocity is proportional to the logarithmic distance from the wall. The buffer layer does not completely follow any of these proportionalities and therefore, establishing the relation between velocity and distance from the wall is difficult for this region. The Spalart-Allmaras model considers all regions of the boundary layer and therefore, careful meshing is required in boundary layers to obtain a converged solution.

2.1.2 k-ε model The k-ε model solves two variables, turbulent kinetic energy and turbulent energy dissipation rate. Two scalar transport equations are solved coupled with the RANS equation to quantify turbulent viscosity which is defined in terms of these two variables. The k-ε model uses wall functions to resolve flow fields near the walls. Wall functions ignore the buffer layer and analytically calculates a nonzero velocity at the walls [6]. This function computes an analytical solution for the viscous sublayer as well and therefore is computationally efficient. However, as the approximated solution is obtained at the walls, the k-ε model is less accurate than Spalart-Allmaras model.

3 Simulation details

The isothermal turbulent flow is modeled using COMSOL Multiphysics software version 5.2. As mentioned earlier, a bottom-up approach is implemented in this systematic study which shows the effect of the boundary layer mesh on the numerical convergence. The effect on numerical convergence can be attributed to the dependence of the first mesh node on the dimensionless distance from the wall in the viscous scale. This dependence varies for different wall boundary conditions such as no-slip condition or wall functions. In the present work, the default wall boundary conditions by COMSOL Multiphysics software for Spalart-Allmaras model (no-slip condition) and k-ε model (wall function) are retained. Figure 1 represents the approach in which the study is developed from simple to complete geometry.

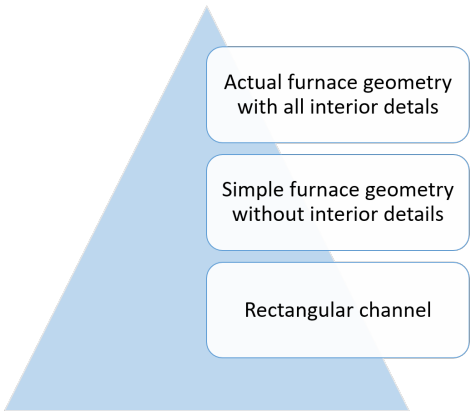


FIGURE 1: Bottom up approach for the study

The boundary conditions for all the three geometries are specified in terms of velocities. For the rectangular channel, air is injected at 1.3 m/s. For the simplified furnace geometry and actual furnace geometry, air and fuel velocities are 1.3 m/s and 5 m/s, respectively. The Reynolds number is such that the flow is in turbulence regime. The effect of boundary layer mesh for both turbulence models is studied for the three geometries that are mentioned in Figure 1. In order to quantify the effect, a non-dimensional distance in viscous units is used. In COMSOL, wall functions are used as wall boundary conditions for the k-ε model. These wall functions are such that the computational domain starts from a distance δ_w from the wall. This distance is known as wall lift-up and a non-dimensional form of this distance in viscous units δ_w^+ is referred as wall lift-up viscous units. On the other hand, the Spalart-Allmaras model uses no-slip boundary condition on the walls. For the Spalart-Allmaras model in COMSOL Multiphysics, a solution is considered to be well resolved if l_c^*, which is, the dimensionless distance to the first mesh cell center from the wall, is close to unity. This paper evaluates the

effect of the boundary layer mesh based on these parameters for the two turbulence models simulated in COMSOL Multiphysics.

4 Results and discussion

The results that are obtained in the present work are divided into three parts according to the level of complexity of geometry as mentioned in Figure 1. It can be observed that there is a dependence of numerical convergence on the boundary layer mesh. This dependence is stronger for the Spalart-Allmaras model as compared to the k-ε model.

4.1 Rectangular channel

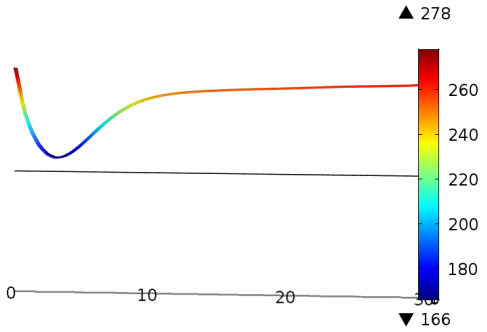
Figure 2 and 3 represent the dimensionless distance in viscous units for the k-ε and Spalart-Allmaras model. The mesh near walls is considered as well resolved if the value of δ_w^+ is close to 11.06 in case of wall functions and l_c^* is close to unity for no-slip boundary condition [7].

The observations from Figures 2 and 3 align with the expected finding that the boundary layer mesh increases the accuracy of the solution. The maximum deviation from the limit of the dimensionless distance for the well-resolved model is observed in the models when the boundary layer mesh is absent (3a and 2a). However, the effect of the absence of the boundary layer mesh on the numerical convergence may differ for the two turbulence models. In the case of k-ε model, this dimensionless distance is not part of the computational domain and therefore may not significantly affect the convergence. Though it decreases the accuracy of the solution. However, in case of the Spalart-Allmaras model, the dimensionless distance to the cell center is part of the computational domain and its higher value suggests that the first mesh node is not in the viscous sub-layer. This may affect the numerical convergence in complex geometries. Therefore, as a next step, the geometry is modified to a simplified geometry of the furnace in which interior details are not included.

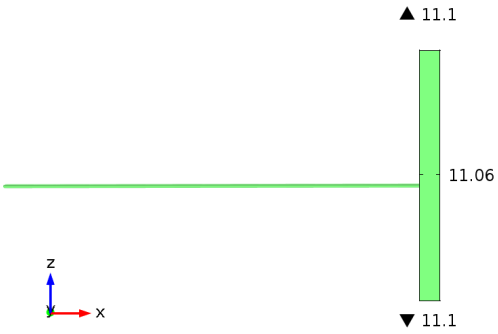
4.2 Simplified geometry

The study of the rectangular channel illustrates the importance of the boundary layer mesh for both the Spalart-Allmaras model and the k-ε model. As a next step, this result is examined on the geometry of the anode baking furnace. However, the actual geometry is simplified by removing baffles and tie-bricks from the interior of the furnace so as to make the model simple for meshing. Figure 4 presents the geometry of the model used as a next step.

For the Spalart-Allmaras model, the presence of the boundary layer highly affects the convergence of the model. Further, Figure 5 presents the dimensionless distance to the cell center for the Spalart-Allmaras model with and without a boundary layer



(a) δ_w^+ across the wall of the rectangular channel model without boundary layer mesh

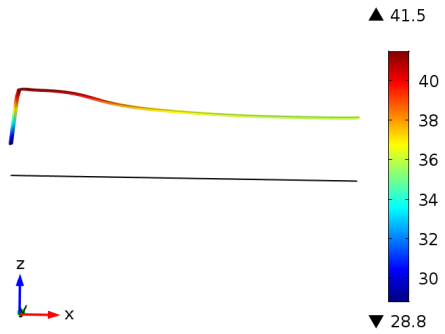


(b) δ_w^+ across the wall of the rectangular channel model with boundary layer mesh

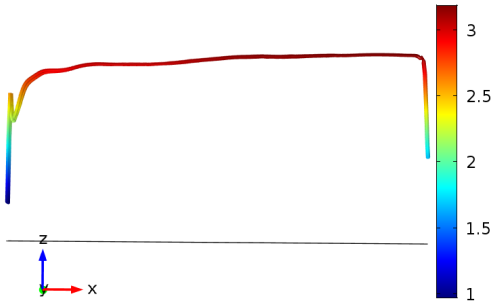
FIGURE 2: δ_w^+ across the wall for k-ε rectangular channel model

mesh. It can be observed that for the model without a boundary layer mesh l_c^* has unrealistically high values. This leads to the divergence of numerical solution of the model. On the other hand, the Spalart-Allmaras model with a boundary layer mesh is refined to such an extent that the highest value of the dimensionless distance to cell center is close to unity.

The effect of the boundary layer meshes on the k-ε model is not significant in terms of numerical convergence. Both the models (with and without boundary layer mesh) are converged. However, a comparison of the wall lift-up viscous units distance, δ_w^+ (Figure 6), shows that the model with a boundary layer mesh is well-resolved while the model without a boundary layer mesh has a significant deviation from the well-resolved model, i.e., δ_w^+ for the model without a boundary layer mesh is significantly large.



(a) Dimensionless distance to cell center across the wall of the rectangular channel model without boundary layer mesh



(b) Dimensionless distance to cell center across the wall of the rectangular channel model with boundary layer mesh

FIGURE 3: Dimensionless distance to cell center across the wall for Spalart-Allmaras simple geometry model

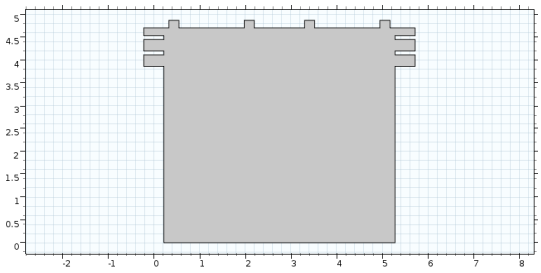
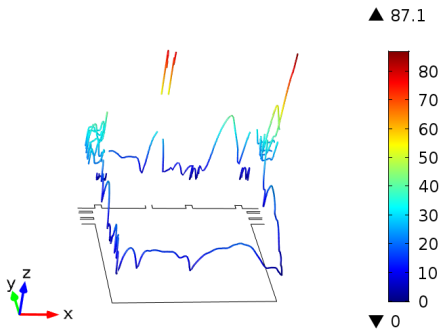


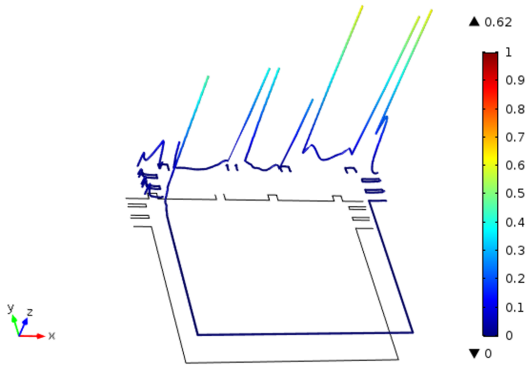
FIGURE 4: Geometry of the anode baking furnace without interior details (size in meters)

4.3 Complete geometry

Analysis of the simple geometry model suggests the effect of the boundary layer mesh similar to the simple rectangular channel. Moreover, it also suggests that the use of a wall function



(a) Dimensionless distance to the cell center across the wall of the simple geometry model without a boundary layer mesh

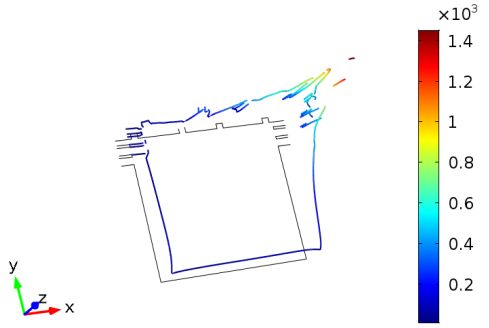


(b) Dimensionless distance to the cell center across the wall of the simple geometry model with a boundary layer mesh

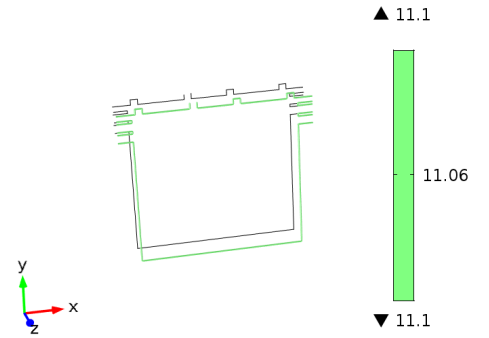
FIGURE 5: Dimensionless distance to the cell center across the wall for the Spalart-Allmaras simple geometry model

boundary condition in the k-ε model facilitates the numerical convergence. Figure 7 shows the geometry of the anode baking furnace with interior details. The meshing of the complete geometry is cumbersome due to the presence of the interior complexity.

Initially, a k-ε model is implemented. The results show that though the model is converged for every type of the mesh, refinement at boundaries is necessary to decrease the wall lift-up viscous scale units which thereby increases the accuracy of the model. One such model is compared with the IB-RAPTOR code. IB-RAPTOR code is an immersed boundary finite volume compressible flow solver that PM2Engineering [8] develops for in-house purposes. The preliminary observations of the velocity profiles developed by COMSOL Multiphysics and IB-RAPTOR code show a good resemblance in developed solutions. However, a detailed investigation of the velocity and the viscosity ratio profile suggests that the solution by COMSOL Multiphysics shows higher fluctuations as compared to IB-RAPTOR code. Figure



(a) δ_w^+ across the wall of the simple geometry model without boundary layer mesh



(b) δ_w^+ across the wall of the simple geometry model with boundary layer mesh

FIGURE 6: δ_w^+ across the wall for k-ε simple geometry model

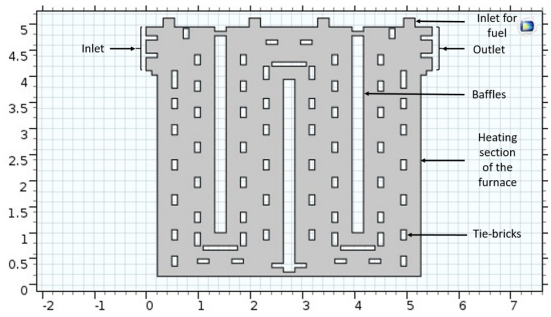


FIGURE 7: A complete geometry of the anode baking furnace with interior details (size in meters)

8 presents the velocity magnitude for two horizontal lines situated at 80.3% (red) and 93.5% (black) from the bottom line of the furnace. Here, the results of the reference code are from the COMSOL Multiphysics software and solid lines represent results from IB-RAPTOR code.

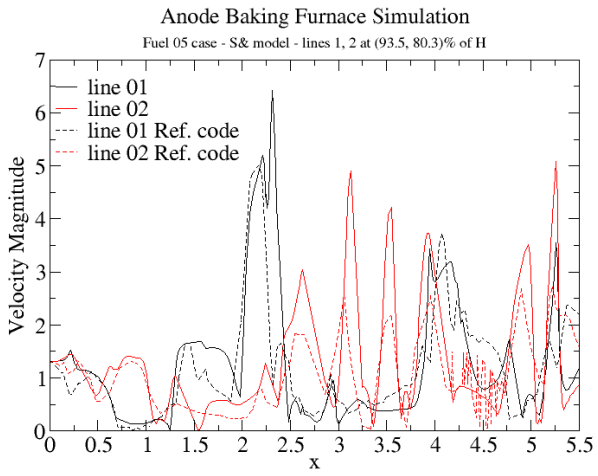
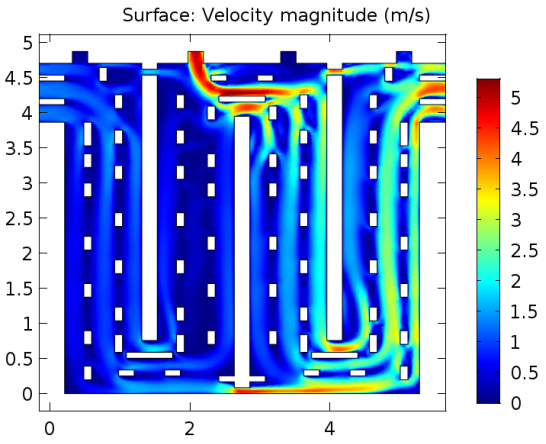


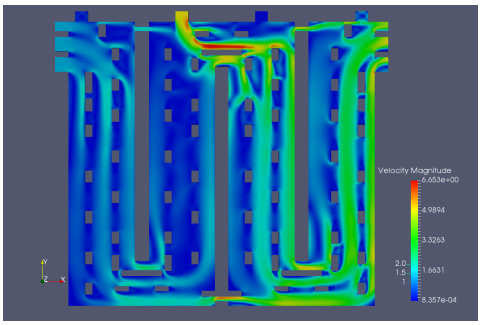
FIGURE 8: A comparison of the velocity magnitude between the solutions computed by COMSOL Multiphysics and IB-RAPTOR code at two horizontal lines situated at 80.3% and 93.5% from the bottom

The overall surface plot of velocity profile developed by COMSOL Multiphysics is also compared with IB-RAPTOR code and is as shown in Figure 9.

Figure 10 indicates the comparison between viscosity ratio at the same lines for different computational codes. A significant difference in terms of viscosity ratios is observed. The possible reasons might be due to the comparison of results of different turbulence model and less refined mesh in case of COMSOL model. The IB-RAPTOR code uses Spalart-Allmaras model with wall functions. However, COMSOL Multiphysics does not allow implementing wall functions to the Spalart-Allmaras model. Therefore, a comparison to a higher extent is possible only if the numerically converged Spalart-Allmaras model is developed. An attempt to develop such numerically converged Spalart-Allmaras model with complete geometry was not successful with the currently available computational power. The analysis of the model with boundary layers and refined mesh at the inlet and outlet shows that the dimensionless distance to the cell center still deviates from unity at certain boundaries. Numerical calculations of the model do not converge due to this deviation. However, the solution after 300 iterations of segregated steps shows a developed velocity profile. Figure 11 indicates the comparison of this developed velocity profile with the IB-RAPTOR code on a horizontal line situated at 93.5% from the bottom. It can be observed that the velocities in x and y-direction are better aligned with



(a) Surface velocity plot developed by COMSOL Multiphysics



(b) Surface velocity plot developed by IB-RAPTOR code

FIGURE 9: Comparison between surface velocity plots developed by COMSOL Multiphysics and IB-RAPTOR code

coarser, medium and finer mesh of IB-RAPTOR model. Figure 12 on the other hand, shows a comparison of the viscosity ratios between two codes and the results significantly deviates indicating that the effect of non-convergence is higher on viscosity ratio. This suggests a need for higher refinement of mesh and thereby requirement of better computational power.

5 Conclusion and remarks

In the present research work, an isothermal turbulent flow in an anode baking process is studied in detail. COMSOL Multiphysics differentiates between two turbulence models namely the Spalart-Allmaras model and the k-ε model based on wall boundary conditions. The Spalart-Allmaras model resolves complete boundary layer whereas, the k-ε model uses wall functions in COMSOL Multiphysics. A systematic model is developed using these two turbulence models, from a simple rectangular channel to a complex anode baking furnace. A mesh sensitivity analysis suggests that a non-dimensional distance in viscous scale units for both turbulence models is close to the accurate wall boundary

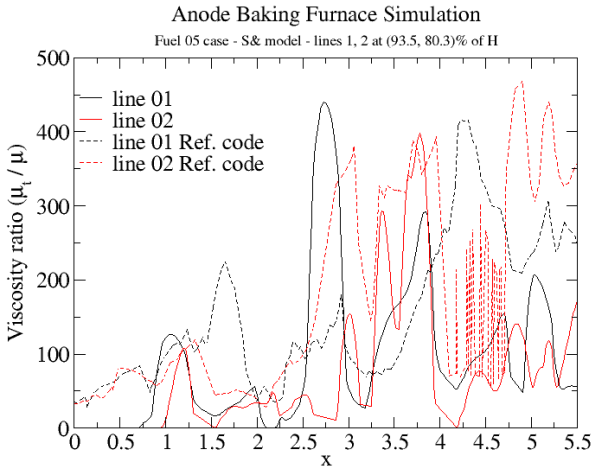


FIGURE 10: A comparison of viscosity ratio between solution developed by COMSOL Multiphysics and IB-RAPTOR code at two horizontal lines situated at 80.3% and 93.5% from the bottom

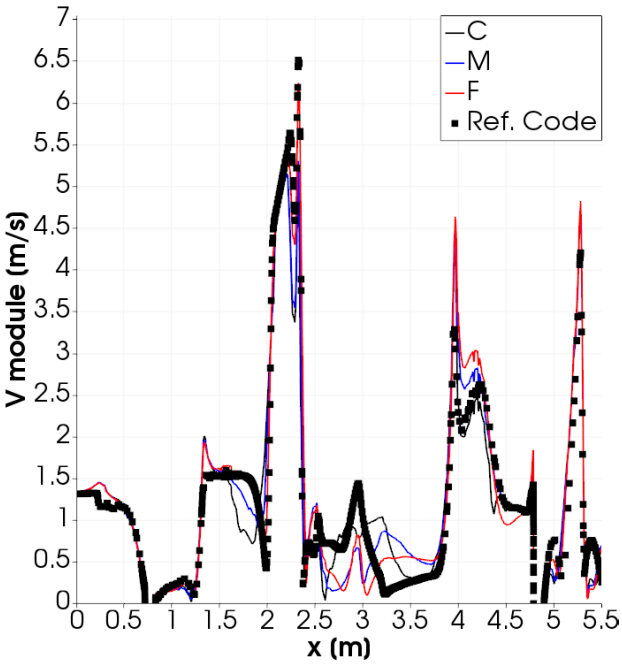


FIGURE 11: A comparison of velocitie magnitude direction between solution computed by refined mesh model of COMSOL Multiphysics and IB-RAPTOR code at a horizontal line situated at 93.5% from the bottom

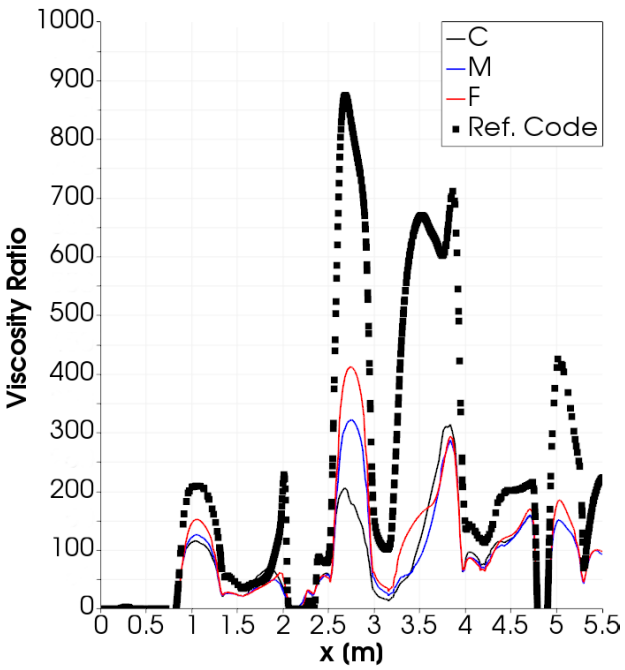


FIGURE 12: A comparison of viscosity ratio between solution computed by refined mesh model of COMSOL Multiphysics and IB-RAPTOR code at a horizontal line situated at 93.5% from the bottom

condition when the boundary layer mesh is included. Therefore, the boundary layer mesh increases the accuracy and possibility of convergence. The dependence of the boundary layer mesh on the numerical convergence is lesser for the k-ε model. However, the boundary layer meshes significantly increase the accuracy of these models. In case of the Spalart-Allamaras model, the numerical convergence is highly dependent on the boundary layer mesh as it decreases the value of the dimensionless distance to the center in the viscous scale to unity. It is difficult to refine the mesh to a higher extent in the complete geometry model due to the interior complexity. This leads to higher dimensionless distance in viscous unit scale in the Spalart-Allmaras model. Therefore, further work is needed to refine the mesh for the complete geometry to have a numerically converged solution.

REFERENCES

[1] Nakate, P., 2017. "Mathematical Modeling of Combustion Reactions in Turbulent Flow of Anode Baking Process". DIAM report 17-10, Delft university of technology.

[2] Severo, D. S., Gusberti, V., Sulger, P. O., Keller, F., and Meier, M. W., 2011. "Recent developments in anode baking furnace design". In *Light Metals 2011*. Springer, pp. 853–858.

[3] Oumarou, N., Kocaefe, D., and Kocaefe, Y., 2018. "An advanced dynamic process model for industrial horizontal anode baking furnace". *Applied Mathematical Modelling,* ***53***, pp. 384–399.

[4] Tajik, A. R., Shamim, T., Al-Rub, R. K. A., and Zaidani, M., 2017. "Two dimensional cfd simulations of a flue-wall in the anode baking furnace for aluminum production". *Energy Procedia,* ***105***, pp. 5134–5139.

[5] Versteeg, H. K., and Malalasekera, W., 2007. *An introduction to computational fluid dynamics: the finite volume method*. Pearson Education.

[6] Frei, W. Which turbulence model should i choose for my cfd application? https://www.comsol.com/blogs/which-turbulence-model-should-choose-cfd-application/.

[7] COMSOLMultiphysics, 2015. "Comsol multiphysics user guide (version 5.2 a)". *COMSOL, AB*, pp. 150–158.

[8] Talice, M., Lampitella, P., and Fiorini, M. Pm2 engineering. https://www.pm2engineering.com/.