Delft University of Technology, Netherlands

DESIGNING AN ENVIRONMENTALLY FRIENDLY ANODE BAKING PROCESS WITH NUMERICAL MODELING

Researchers at Delft University of Technology in the Netherlands are using multiphysics simulation to design an environmentally friendly anode baking process in collaboration with Aluchemie, an anode production company.

by RACHEL KEATLEY

FIGURE 1 Anode baking furnace at Aluchemie.

Aluminum, the third most abundant element in the Earth's crust, can be found in everything from the foil holding last night's dinner leftovers to the fuselage of a plane traveling across the world. Before aluminum can be used to produce such a variety of items, it has to be smelted and extracted through the Hall–Héroult process. During this process, aluminum is removed from an aluminum-rich rock, bauxite, using green anodes. In order to be effective in the Hall–Héroult process, green anodes need to have a low reactivity and a high strength and conductivity. To obtain these qualities, the anodes need to be baked.

Prajakta Nakate, a PhD student at Delft University of Technology (TU Delft), is part of a research team that is studying the design of the anode baking process. This project is in collaboration with Aluchemie, a carbon anode baking company in the Netherlands. To understand and optimize the anode baking process for increased aluminum production, the team turned to numerical simulation.

» AN ANODE BAKING PROCESS FIT FOR A CHEF

When baking a cake, a variety of ingredients are needed in order to get the right consistency, texture, and flavor. Think of the anode baking process like baking a cake, except the ingredients consist of multiphysics phenomena, such as turbulent flow, combustion processes, conjugate heat transfer, and radiation — and instead of a well-baked pastry, the end product is anodes that can be used in the Hall–Héroult process for aluminum extraction. "I was mainly interested in this project because it is a multiphysics problem," said Nakate. Unlike baking a cake, the anode baking process strives to achieve multiple goals, including uniform heat, reduced energy usage, and decreased soot formation during combustion.

This anode baking process is extremely energy intensive and releases environmentally dangerous emissions, like nitrogen oxides (NOx). This toxic gas is a common air pollutant and can form smog and acid rain. Nakate's research focuses on the reduction of NOx emitted during the anode baking process to limit the negative harmful effects the process has on the environment. "When it comes to environmental studies, chemical processes always get blamed, and that is what motivated me to work on the optimization of the anode baking process and ensure that it has minimal environmental impact," said Nakate.

In order to decrease the formation of NOx during anode baking, it is important to first understand all of the parameters involved in the process. Nakate said, "To understand all these things, you need a more sophisticated approach, and having a mathematical model to understand these parameters is the best choice."

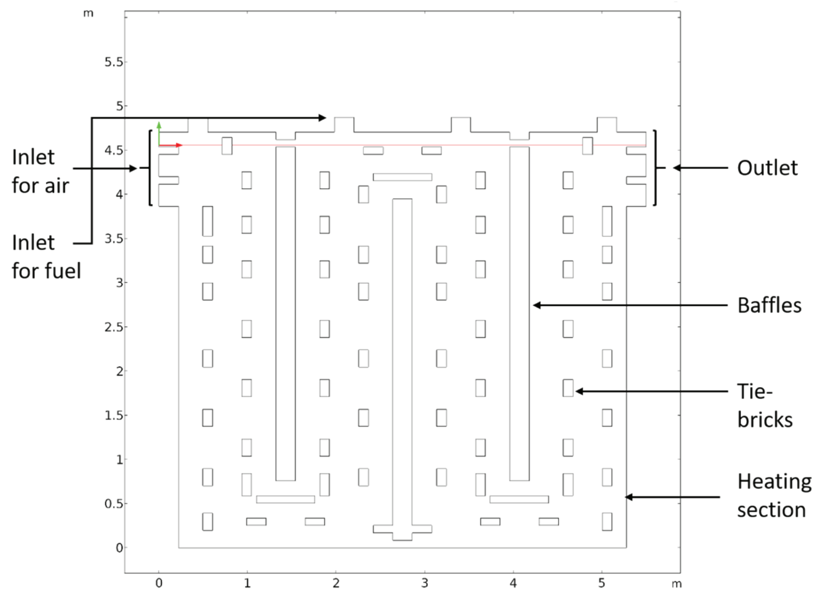
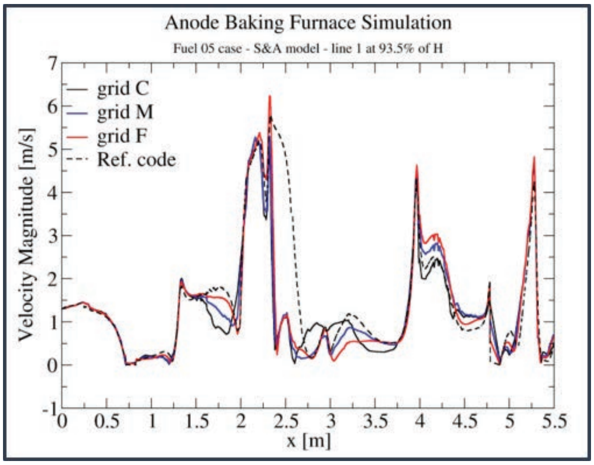


FIGURE 2 Geometry along with the boundaries of the anode baking furnace modeled in COMSOL Multiphysics®. (The most important parts of the furnace are below the horizontal red line.)

» NUMERICAL MODELING: THE SECRET INGREDIENT TO DESIGNING AN IDEAL ANODE BAKING PROCESS

Prior to teaming up with TU Delft, Aluchemie tried to optimize their anode baking furnaces (Figure 1) using trial and error, but this method proved to be time consuming. "The most important part of this project is to identify the anode baking process's problem areas, and I would say that is only possible with simulation," said Nakate. When it came to modeling the anode baking process, the TU Delft research team used the COMSOL Multiphysics® software because it provides a multiphysics environment, which is essential for this particular project.

The researchers studied the anode baking process using two



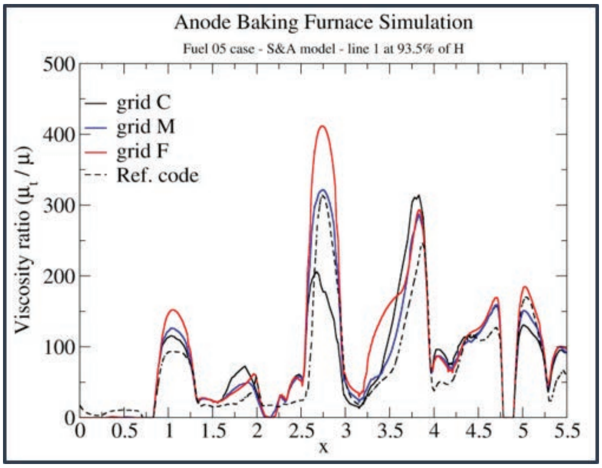


FIGURE 3 Comparison of COMSOL Multiphysics® and IB Raptor code's simulation results for velocity (left) and viscosity ratio (right).

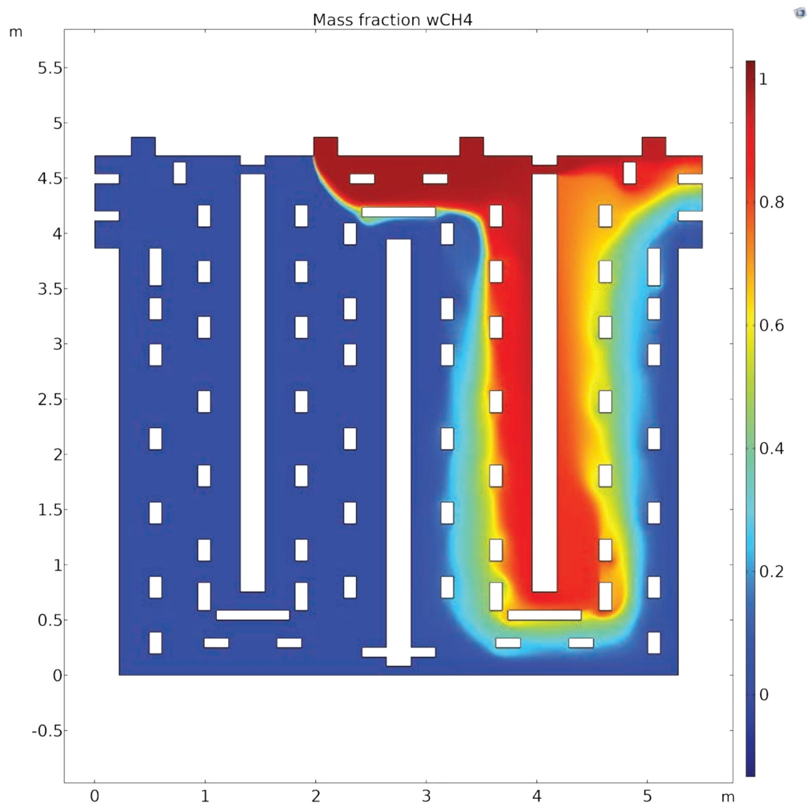


FIGURE 4 Mass fraction of CH_4 in the reactive turbulent flow model.

models. The first model analyzed a nonreactive turbulent flow of air and fuel (methane) in the furnace, while the second model analyzed a reactive flow with radiation in the furnace. The second model was also a continuation of the first model. The multiple physical phenomena involved in the anode baking process were described in a model that translates into a set of mathematical equations, which formed the basis of these numerical models.

Both models included the same geometry: a 2D section from a furnace's heating zone (Figure 2). According to Nakate, working with the complex geometry was one of the most challenging aspects of this project. The geometry of the furnace includes 3 baffles and about 60–70 tie-bricks in each section of the furnace. "If you replace the ties at different positions, they change the flow in the furnace, which affects the anode baking process's chemical species distribution and temperature," said Nakate. The tie-bricks and baffles provide structural strength to the furnace's flue wall from which the furnace's exhaust is released.

» NONREACTIVE AND REACTIVE TURBULENT FLOW MODELS

When working on the nonreactive turbulent flow model, Nakate and the team simulated and compared two turbulent flow models: the Spalart–Allmaras model and the k-ε model. Both of these models have their own advantages, especially in relation to analyzing anode baking.

The team validated the flow field results generated by the Spalart–Allmaras model with the IB Raptor code provided via another simulation environment. "The IB Raptor code is mostly a flow solver; we wanted to validate our results to a software that is dedicated to flow simulations," said Nakate. COMSOL Multiphysics and the IB Raptor code generated similar velocity and viscosity flow results in the furnace (Figure 3).

The research team extended the first model by adding a single step combustion reaction of methane (CH_4) and heat transfer, including radiation in participating media, using the Chemical Reaction Engineering Module and the Heat Transfer Module, add-on products to COMSOL Multiphysics, respectively. The simulation results of the reactive flow model with radiation provided the team with reasonable results (Figure 4). This opens to further improvements of the models for more understanding and optimization of NOx furnaces.

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>
> — PRAJAKTA NAKATE, TU DELFT

» COOKING UP NEW MODELS FOR ANODE BAKING RESEARCH

Simulation enabled the TU Delft team and Nakate to analyze and identify important regions in the anode baking furnace, which would not have been possible with experimentation alone due to the furnace's large size. "We can only see the furnace from the top by removing the burner and taking photographs with the thermal camera, but viewing the actual temperature or the actual chemical species distribution in the furnace is only possible with simulation," said Nakate.

As for future research, the TU Delft team is currently working on extending their anode baking process's 2D model to a 3D transient model. They also plan to thoroughly investigate combustion in their new model, which will help them learn more about NOx reduction in the anode baking process. Radiation, a primary physical phenomenon in the anode baking process, will also be further analyzed in the extended model.

While discussing her own personal goals, Nakate said: "I wanted to work on a project that had a direct application to industries and a positive environmental impact." Therefore, studying the anode baking process alongside Aluchemie was a perfect combination of her goals. With the knowledge gained, the TU Delft team and Nakate are confident about continuing their research and finding new ways to design an optimized anode baking process with simulation. ◎