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Comparison of three combustion models for simulating anode baking furnaces



François Grégoire^{a,b}, Louis Gosselin^{a,b,*}

^a Department of Mechanical Engineering, Université Laval, Québec City, Québec, Canada
^b Aluminium Research Centre - REGAL, Canada

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<i>Keywords:</i> Hall-Héroult process Anode baking Furnace Combustion models	Carbon anode blocks used in the Hall-Héroult process for primary aluminum production have to be baked up to 1100 °C in dedicated furnaces. These furnaces are equipped with burner ramps to heat the air circulating in the flues at 1200 °C, so that the anodes reach the required temperature. It is therefore mandatory to include the heat provided by the burners in a numerical model of an anode baking furnace. In this work, we modeled the heat input at the burners in three ways: the Eddy-Dissipation model, the Mixture Fraction/PDF approach and a simplified approach consisting in injecting an equivalent calorific value at the burners' inlets. Results obtained with the first two models are very similar in terms of anode baking prediction but slightly different in terms of flame temperature prediction. Results obtained with the simplified approach show that the model can replace combustion model to predict anode baking, but calibration of boundary conditions is necessary in order to match more elaborate combustion models. The importance of other elements of the model in the flue channel of the furnace has been verified: radiation (cannot be ignored, large influence on the spatial temperature distribution), heat transfer due to species diffusion (negligible influence on the baking, but slight effect on flame shape and temperature), and buoyancy (no significant effect on the results in the furnace firing sections).

1. Introduction

According to the International Aluminum Institute, the global primary aluminum industry produced approximately 50 million metric tons of new aluminum in 2013. All of this production is achieved with the Hall-Héroult process, the most efficient version of which relies on the use of prebaked carbon anode blocks within electrolysis cells operating at about 960 °C. In short, the dissolved alumina (Al₂O₃) in the cell reacts with the carbon of the anode blocks to form CO and CO₂, and as a result, pure aluminum is obtained. Therefore, the aluminum industry is constantly consuming carbon in order to produce aluminum. A typical carbon consumption rate is 0.5 ton for each ton of aluminum produced, representing approximately 15–20% of the overall production costs of an aluminum smelter [1].

The carbon anode quality is of prime importance for the profitability of an aluminum plant. Variability of key anode properties such as density, electrical resistivity, permeability, thermal shock resistance and mechanical strength have a profound influence on the stability and the costs of the electrolysis process. For example, a higher anode permeability will increase the transport of oxidant gases (air and CO₂) within the anode matrix, therefore increasing the anode consumption in the electrolysis cell, resulting in a shorter anode lifetime and higher carbon consumption [2]. Aluminum smelters are continuously seeking for new ways to improve anode fabrication, from the supply of raw materials to the optimization of the different production steps.

Prior to their use in an electrolysis cell, the carbon anode blocks are fabricated in 4 main steps. First, the paste production consists in the mixing of raw materials, the typical recipe being 65% petroleum coke, 15% binder pitch and 20% recycled anode butts. The next step is to form the mixed paste into blocks by moulding or vibrocompaction, resulting in what are called green anodes. The third step consists in baking the anodes in a furnace where they will reach a maximum temperature of about 1100 °C in order to acquire adequate chemical, electrical, mechanical and thermal properties. Finally, the last sept of the anode fabrication is the rodding, which consists in equipping the baked anodes with an assembly that enables the carbon blocks to be held in cells and through which the electric current passes.

The baking of the anodes is the most expensive and the most energyconsuming step of the anode fabrication process [1]. The anodes are baked in large furnaces that steadily burn natural gas (or oil) to generate enough heat for the baking process to take place. The energy efficiency of anode baking furnaces (ABF) is a primary concern in the

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^{*} Corresponding author. Department of Mechanical Engineering, Université Laval, Québec City, Québec, Canada. *E-mail address:* Louis.Gosselin@gmc.ulaval.ca (L. Gosselin).

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Nomenclature		
a to j	Molar coefficients	
2	Constant of the Eddy-Dissipation model	
	Turbulence model coefficient and constant, respectively	
	Mixture fraction model constants	
C_d, C_g C_p	Heat capacity $[J kg^{-1} K^{-1}]$	
$D_{i,m}$	Diffusion coefficient of species <i>i</i> in mixture $[m^2 s^{-1}]$	
$D_{i,m}$ f, f'^2	Mixture fraction, mixture fraction variance	
g	Gravitational acceleration [m s ⁻²]	
h, h_i , $h_{s,i}$, $h_{f,i}^0$ Enthalpy [J kg ⁻¹]		
Ι	Radiative intensity $[W m^{-2} sr^{-1}]$	
k	Turbulent kinetic energy [J kg ^{-1} or m ^{2} s ^{-2}]	
'n	Mass flow rate [kg s ⁻¹]	
Μ	Molecular weight $[g \text{ mol}^{-1}]$	
р	Pressure [Pa]	
P_k, P_b		
Pr_t	Turbulent Prandtl number	
Q	Heat of reaction $[J kg^{-1}]$	
$\begin{array}{c} Q\\ \dot{Q}\\ \overrightarrow{r} \end{array}$	Source term [W m ⁻³]	
r R	Position vector $P_{\text{restrict}} = 1$	
K D	Reaction rate [kg $m^{-3} s^{-1}$] Universal gas constant [J $mol^{-1} K^{-1}$]	
$\frac{R_u}{\overrightarrow{s}}$	Unit direction vector	
S		
S Sc _t	Modulus of the mean rate-of-strain tensor $[s^{-1}]$ Turbulent Schmidt number	
u sct	Velocity components $[m s^{-1}]$	
	Time [s]	
T, T _{ref}	Temperature [°C]	
1, 1 ref	remperature [0]	

aluminum industry, typically expressed in the amount of energy that an ABF consumes per ton of baked anodes produced (GJ/ton). Recent furnaces consume about 2 GJ/ton [1]. In addition to energy consumption, the ABFs constantly need to be serviced with new refractories and cleaned between baking cycles so that the baking process remains uniform and safe.

Numerical modeling of the anode baking process started in the early 1980s. The need for numerical models came naturally since proceeding by 'trial and error' experiments on a furnace is time and resource consuming due to the length of the baking cycle and the severe temperature conditions in the furnace. Moreover, the quality of several hundreds of anodes could be jeopardized with in-situ optimization of a furnace. Complexity and applications of ABF numerical models vary a lot, but they can be separated in two main categories: process models and design models.

The application of process models is to predict the overall conditions in the furnace during an entire baking cycle. These models are one or two-dimensional and they essentially solve momentum and energy balances along the flue channel, accompanied by the conduction equation in a certain number of slices of the solids (anodes, coke, refractories) to determine their temperature. The flue gas and the solids are coupled at the flue wall, interacting with heat flux or temperature boundary conditions. Sub-models are used to calculate the volatile release from the anodes, air infiltration/exfiltration through the top of the furnace and heat losses to environment and foundation. The furnace is treated as a counterflow heat exchanger where the gas is flowing from blowing ramp to exhaust ramp and the solids are "marching" in the opposite way at the average displacement speed of the equipment on the furnace (blower ramps, burner ramps, exhaust ramp, etc.). A complete description of that kind of model and underlying algorithm can be found in Ref. [3]. The process models are computationally cheap and give the whole portrait of the baking cycle with the help of just a few boundary conditions needed at each end of the furnace. Their shortcoming is that they do not provide detailed results of the anode baking

x	Cartesian coordinates [m]	
Х	Heating value [J kg ⁻¹]	
у	Mass fraction	
Greek letters		
δ_{ij}	Kronecker delta	
ε	Dissipation rate of turbulent energy $[m^2 s^{-3}]$	
κ	Absorption coefficient $[m^{-1}]$	
λ	Thermal conductivity [W $m^{-1} K^{-1}$]	
μ	Dynamic viscosity [Pa s]	
μ_t	Turbulent viscosity [Pa s]	
ν	Kinematic viscosity $[m^2 s^{-1}]$ or stoichiometric coefficient	
ρ	Density [kg m ⁻³]	
σ	Stefan-Boltzmann constant [W m ⁻² K ⁻⁴]	
σ_k, σ_e	Turbulence model constants	
σ_t	Mixture fraction model constant	
Ω	Control angle [sr]	
Subscripts		
coarse	Refers to coarse mesh	
comb	Refers to combustion	
fine	Refers to fine mesh	
i, j	Species	
i, j, l	Refers to cartesian coordinates x , y or z	
rad	Refers to radiation	

in space and time. In particular, they do not provide a tridimensional temperature portrait of the anode stack in the pit, and the flow in the flue channel is largely simplified to that in an equivalent duct. Nevertheless, with the always increasing performance of computers, the flue gas flow can be modeled as a two-dimensional duct flow as described recently in Ref. [4].

The design models are two or tridimensional models that aim at capturing the space and time variations of the most important phenomena that take place during the baking process: convective, diffusive and radiative heat transfer, combustion of natural gas (or fuel) and volatiles in the flue channel, distribution of the turbulent gas flow in the flue channel, evolution of key anode properties, etc. Instead of including the geometry of the whole baking cycle in the model, which would be computationally expensive, the design models only include one stack of anodes and the corresponding coke, refractories and flue channel. Symmetry planes are presumed at the center planes of the anodes and flue channel. The design models consist mainly in a set of coupled partial differential equations for the gas and solids: continuity equation, momentum equations, turbulence model, species transport equations (the number of species depending on the complexity of the combustion model, typically 4-6 species), energy equation, radiation model and pitch pyrolysis kinetics equations. These models rely mostly on known boundary conditions at the inlet of the flue channel which are usually obtained with the help of a process model for the whole baking cycle, but can also be obtained through measurement campaigns in the furnace. This kind of model is necessary in order to optimize the geometry of a furnace or a detailed operational condition of the furnace (e.g., adjust the flame length at the burners). The shortcoming of the design models is their significant computational requirements, especially if implemented in three dimensions since the model can easily contain over 10 unknown variables to solve. A typical example of a tridimensional design model can be found in Ref. [5].

Combustion modeling is a crucial aspect of a design model. In the past, authors have used either the Eddy-Dissipation model [5], which is

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