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Uwe Janoske (Hrsg.)

Varchasvi Lakshmi Nandana

DEVELOPMENT OF A NUMERICAL MODEL TO STUDY THE ELECTRIC AND THERMAL BEHAVIOUR OF A HALL-HÉROULT CELL

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Development of a Numerical Model to Study the Electric and Thermal Behaviour of a Hall-Héroult Cell

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Abstract

Aluminium is one of the most widely used metals in the world. The production of primary aluminium is a complex process with high energy requirements. Climate goals have steered many countries to shift towards renewable sources for electricity production, increasing the energy costs. The transition necessitates smelters to augment the production efficiency to produce aluminium at competitive prices. Additionally, the fluctuations in the electricity price in the energy market could be utilized to benefit the smelter by achieving flexibility in the production process. A detailed understanding of the cell behaviour is necessary to realize these objectives. The corrosive environment and high temperatures inside the Hall-Héroult cell, as well as the high magnetic fields, significantly reduces the observability of the process, as measurement-based research is significantly restricted. A numerical model, on the other hand, provides several advantages to study the influence of various cell parameters without affecting industrial production.

The thermal balance of the cell is critical to achieving stable and efficient production. In the present work, a numerical model in the Multi-Region framework is developed to study the electric and thermal behaviour of the cell. The numerical model is developed in OpenFOAM® 4.0, an open-source CFD toolkit.

The numerical model is validated by comparing the simulation predictions with the industrial measurements. This is followed by studying the influence of the operational parameters on the electric and thermal behaviour of the cell. The operational parameters considered in this study are the amount of aluminium and electrolyte, anode-to-cathode distance, cell current, bath composition and sidewall cooling. The influence on the cell behaviour is evaluated by analyzing the variation in the ledge thickness, the bath temperature, the ohmic voltage and the cell specific energy consumption. The results of this work provide detailed insights into the thermoelectric behaviour of the cell and identifies critical parameters, which has a high impact on the production efficiency.

Kurzfassung

Aluminium ist eines der auf der Welt am häufigsten verwendeten Metalle. Die Herstellung von Primäraluminium ist allerdings ein komplexer Prozess mit hohem Energiebedarf. Wegen der Klimaziele haben viele Länder entschieden, bei der Stromerzeugung auf erneuerbare Energien umzusteigen, was die Energiekosten steigen lässt. Um Aluminium dort weiterhin zu wettbewerbsfähigen Preisen produzieren zu können, müssen die Aluminiumhütten die Effizienz und Flexibilität der Zellen steigern. Um diese Ziele zu erreichen, ist ein detailliertes Verständnis des Verhaltens der Aluminiumzelle erforderlich. Eine korrosive Umgebung, hohe Temperaturen sowie starke Magnetfelder schränken die Beobachtbarkeit des Prozesses in der Hall-Héroult-Zelle stark ein. Die oben genannten Ziele können daher allenfalls ansatzweise über Messungen erreicht werden. Ein numerisches Modell zur Untersuchung des Einflusses verschiedener Zellparameter, bietet hier mehrere Vorteile ohne dabei die industrielle Produktion zu beeinträchtigen.

Einer den entscheidenden Faktoren fur eine stabile und effiziente Produktion ist die thermische Bilanz einer Hall-Héroult-Zelle. In der vorliegenden Arbeit wird ein numerisches Modell, basierend auf dem Multi-Region Framework des OpenFOAM® 4.0 entwickelt, um das elektrische und thermische Verhalten der Zelle zu untersuchen.

Die Simulationsvorhersagen werden mit industriellen Messungen verglichen, um das numerische Modell zu validieren. Im Anschluss wird der Einfluss verschiedener Betriebsparameter auf das elektrische und thermische Verhalten der Zelle untersucht. In dieser Studie werden dazu die folgenden Betriebsparameter variiert: die Menge an Aluminium und Elektrolyt, der Abstand zwischen Anode und Kathode, der Strom durch die Zelle, die Zusammensetzung des Elektrolyts und die Seitenwandkuhlung. Der Einfluss dieser Betriebsparameter auf das Verhalten der Zelle wird durch die Analyse der Schwankungen der Dicke der Randkruste, der Elektrolyttemperatur und der ohmschen Spannung bewertet. Die Ergebnisse dieser Arbeit geben einen detaillierten Einblick in das thermoelektrische Verhalten der Zelle und zeigen kritische Parameter auf, die einen großen Einfluss auf die Produktionseffizienz haben.

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Nomenclature

Acronyms

Symbol	Description	Units
ACD	Anode-to-Cathode distance	–
CFD	Computational fluid dynamics	–
CV	Control volumes	–
$MULES$	Multidimensional Universal Limiter for Explicit Solution	–
PID	Proportional-integral-derivative	–
$PISO$	Pressure-Implicit with Splitting of Operators	–
PCM	Phase change material	–
$RANS$	Reynolds-averaged Navier-Stokes	–
RNG	Re-Normalisation Group	–
SHE	Shell heat exchanger	–
$SIMPLE$	Semi-Implicit Method for Pressure Linked Equations	–
VOF	Volume of Fluid	–

Dimensionless numbers

Symbol	Description	Units
Gr	Grashof number	–
Nu	Nusselt number	–
Pr	Prandtl number	–
Ra	Rayleigh number	–

Greek Symbols

Symbol	Description	Units
α	Volume fraction	–
β	Thermal coefficient of volume expansion	–
γ	Melt fraction	–
Γ	Interface	–
δ	Cell-center to face-center distance	m
ϵ	Small numerical constant	–
ε	Thermal emissivity constant	–
η	Overvoltage	$\mathrm{kg\,m^2/(s^3\,A)}$
θ	Function for Boussinesq term	–
λ	Convection cooling coefficient	$\mathrm{kg/(s^3\,K)}$
μ	Mixture dynamic viscosity	$\mathrm{kg/(m\,s)}$
ξ_{ag}	Anode gas bubbles depth	m
ξ_b	Anode-to-cathode distance	m
ϖ_{ag}	Anode surface coverage of gases	–
ρ	Mixture density	$\mathrm{kg/m^3}$
σ_e	Electric conduction coefficient	$\mathrm{s^3\,A^2/(kg\,m^3)}$
ς_c	Cell current efficiency	–
ϕ	Electric potential	$\mathrm{kg\,m^2/(s^3\,A)}$
χ	Cell specific energy	$\mathrm{m^2/s^2}$
ψ	Solid fraction	–

Roman Symbols

Symbol	Description	Units
C_p	Mixture specific heat capacity	$\mathrm{m^2/(K\,s^2)}$
C	Carman-Kozeny constant	1/s
$\mathbf{E}$	Electric field	$\mathrm{m\,kg/(s^3\,A)}$
g	Melt fraction update function	–
$\mathbf{g}$	Gravitational acceleration	$\mathrm{m/s^2}$
ΔG°	Standard Gibbs energy of the reaction	$\mathrm{kg\,m^2/(s^2\,mol)}$
h	Specific enthalpy	$\mathrm{m^2/s^2}$
ΔH	Standard enthalpy change	$\mathrm{m^2/s^2}$

j	Electric current density magnitude	$\mathrm{A/m^2}$
$\mathbf{J}$	Electric current density vector	$\mathrm{A/m^2}$
k	Mixture thermal conduction coefficient	$\mathrm{kg\,m/(s^3\,K)}$
l	Characteristic length	m
L	Latent heat of melting	$\mathrm{m^2/s^2}$
q	Heat flux	$\mathrm{kg/s^3}$
S_D	Momentum source	$\mathrm{kg/(m^2\,s^2)}$
S_ohm	Volumetric heat source	$\mathrm{kg/(m\,s^3)}$
T	Temperature	K
T_s	Solidus temperature	K
T_l	Liquidus temperature	K
$\mathbf{u}$	Velocity vector	m/s
U	Voltage	$\mathrm{kg\,m^2/(s^3\,A)}$

subscripts

Symbol	**Description**	**Units**
aa	Reaction overvoltage at the anode	–
ac	Concentration overvoltage at the anode	–
ag	Anode gas	–
amb	Ambient	–
alu	Aluminium	–
b	Bath	–
c	Current	–
cc	Concentration overvoltage at the cathode	–
e	Electric	–
en	Enhanced	–
eff	Effective	–
ext	External	–
f	Fluid	–
$ledge$	Ledge	–
ohm	Ohmic	–
r	Radiative	–
s	Solid	–
w	Wall surface	–

superscripts

Symbol	Description	Units
rev	Reversible	–

Universal constants

Symbol	Description	Units
F	Faraday constant	$\mathrm{s\,A/mol}$
R	Universal gas constant	$\mathrm{kg\,m^2/(s^2\,K\,mol)}$
ϑ	Stefan-Boltzmann constant	$\mathrm{kg/(s^4\,K)}$