Three-Dimensional Steady State Multiphysics CFD Modeling of a Novel Aluminium Reactor

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Carbothermic reduction is a nontraditional chemical process for aluminium production, based on the endothermic chemical reduction reaction occuring between aluminium oxide and carbon. This process has potential for drastic reduction of fixed and operation costs of the investment. Furthermore, it is environmentally benign and more energy-efficient, having been identified and extensively investigated as a potential alternative to Hall-Heroult electrochemical reduction. Nonetheless, its remarkable complexity poses technical obstacles to efficient implementation. The ARP carbothermic aluminium reactor (Johansen and Aune, 2002) is aimed at achieving reactor scaleup but involves many modeling, simulation, experimentation and design challenges. Actual carbothermic reduction of alumina occurs in the second stage of this multiphase reactor: a high-temperature molten slag formed at a temperature of ca. 1950 °C (1st stage) is fed into a submerged arc furnace (2nd stage), where it reacts at a temperature of ca. 2050 °C to CO and Al. Previously published process and CFD modeling studies (Gerogiorgis and Ydstie, 2003, 2004) have contributed to our understanding of heat effects, flow patterns and crucial design variables.

Multiphysics 3D CFD modeling of the ARP reactor core stage with a focus on visualizing and understanding the complex multiphase flow therein can greatly benefit reactor design and capitalize on our previous successful computer modeling efforts. The interaction among Joule heating, endothermic reaction, slag convection and gas dispersion phenomena governs reactor performance, so the quintuple PDE problem (electric charge, heat, momentum and gas fraction balances) for the slag flow is solved via a commercial finite element solver (FEMLAB® v. 3.0), to obtain potential, temperature, velocity and gas fraction 3D distributions in the reactor domain.

Multiphysics 3D CFD models in FEMLAB feature many attractive characteristics:
(a) Geometry can be parameterized to match the dimensional design changes
(b) Discretization is adjustable, to probe bulk (slag flow) and local (gas production) phenomena
(c) They can correspond to isothermal flow (water modeling), eliminating Joule electric heating
(d) They can benefit from quantitative water modeling experimentation
(e) They can be parameterized to simulate various reactor operation modes

This multiphysics CFD study provides reactor design guidelines by computing realistic slag flow velocity and gas volume fraction distributions via explicit three-dimensional PDE formulations; the latter can be parameterized against experimental data obtained from physical water modeling. A sensitivity analysis of flow with respect to gas injection fluxes is also performed in order to analyze the effect of gas production on the macroscopic form and stability of the two-phase flow. The multiphase CFD simulation results obtained here are furthermore compared to experimental observations and results from an ARP physical model constructed at the ALCOA Technical Center.