MULTISCALE MODELING FOR ELECTRODE VOLTAGE OPTIMIZATION IN THE DESIGN OF A CARBOTHERMIC ALUMINIUM PROCESS

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Abstract

Multiscale modeling is a tool aimed at combining mathematical descriptions of different process scales into properly tailored scale integration hierarchies facilitating design-relevant modeling and simulation. This concept has been successfully applied in deriving state variable distributions of complex processes; in a relevant paper, we discuss its implementation in the field of carbothermic aluminium production. The three-level multiscale model proposed therein (Gerogiorgis and Ydstie, 2003a) is aimed at deriving state variable profiles for a conceptual high-temperature multiphase carbothermic aluminium reactor, its objective being to simultaneously solve the electric charge, heat, momentum, mass and molar balances and hence enhance our understanding of this spatially distributed, endothermic electrochemical process. The present paper presents our work on reactor electrode voltage optimization via MINLP modeling and validates the suitability of this approach via explicit two-dimensional multiphase flow CFD modeling.

Keywords

Multiscale process modeling, MINLP, computational fluid dynamics (CFD), carbothermic aluminium.

Introduction

The integration of Computer-Aided Process Design and Computational Fluid Dynamics is a research objective that receives ever-increasing attention and promises accurate simulation of complex large-scale PDE design problems which arise in cutting-edge chemical process applications. Multiscale model representations of challenging processes have emerged as a powerful idea for efficient simulations. Atmospheric pollution modeling, advanced materials and CAD of multiphase flow unit operations are all fields in which multiscale modeling has been already successful (Gerogiorgis and Ydstie, 2003a – and references therein). The reviews of Maroudas (2000) and Pantelides (2000) provide remarkably thorough discussions of challenges. Novel developments in the field include the multiscale hierarchical modeling (Raimondeau and Vlachos, 2002), the wavelet-based adaptive multiscale simulation of dynamic process systems (Bindal et al., 2003) and the object-oriented multizonal modeling (Bezzo et al., 2003).

Multiscale modeling is important for process design inasmuch as (a) ab initio molecular/microscale simulation is essential in order to derive the macroscopic properties, (b) standard modeling simplifications are not admissible because of inherent limitations to physical understanding, sharp model nonlinearities, high accuracy requirements, poorly parameterized phenomenological source equations, or infeasible, inadequate or inconclusive experimentation, (c) direct computer simulation is prohibitively expensive.

The multiscale model that has been proposed for the ARP carbothermic reactor (Johansen and Aune, 2002) and presented in our paper (Gerogiorgis and Ydstie, 2003a) is motivated by many of the foregoing limitation factors as elaborated elsewhere (Gerogiorgis and Ydstie, 2003b). The ongoing multiscale modeling effort has benefited a lot from our previous reactor-section CFD sensitivity analyses and also by the full-reactor multiphysics CFD simulations already published (Gerogiorgis and Ydstie, 2003c, 2004).

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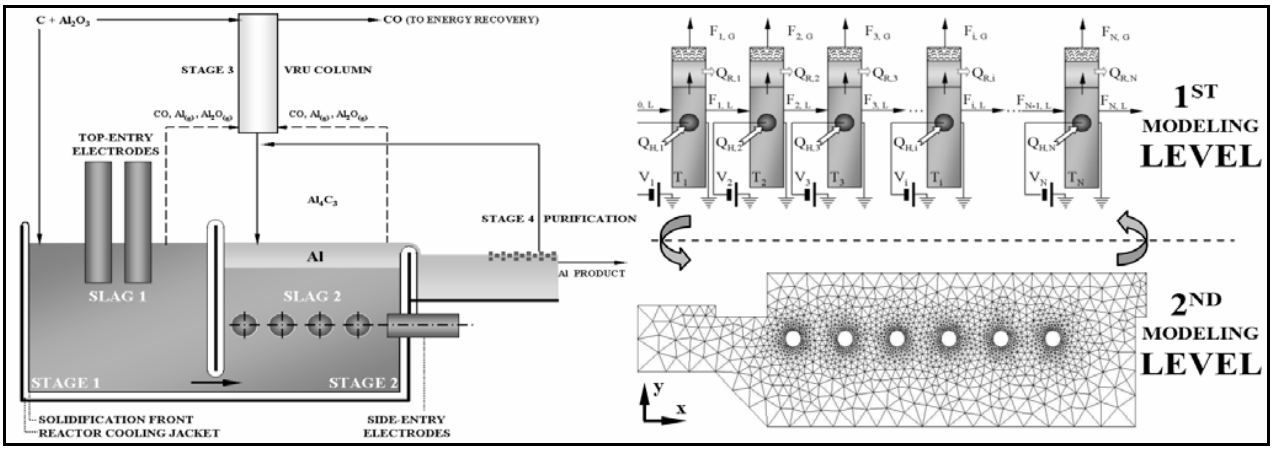

Figure 1: The ARP carbothermic reactor (Johansen and Aune, 2002) and the computational domain discretizations.

Carbothermic Process Modeling

Carbothermic Al production is an environmentally benign process with a potential for industrial application. The conceptual multistage electrothermic reactor patent of ALCOA and ELKEM (Johansen and Aune, 2002) aims at increased volumetric production via scaled-up reactors; a schematic of the ARP concept is presented in Figure 1. The distributed nature of this configuration poses several technical challenges (Gerogiorgis and Ydstie, 2003c). Distributed Joule heating (achieved by independent AC electrode pairs) is necessary for the endothermic reaction. The voltage imposed on electrodes has been confirmed as the most suitable design variable by elaborate steady state CFD sensitivity analyses (Gerogiorgis and Ydstie, 2003c). Electrode voltage optimization has been already addressed recently (Gerogiorgis and Ydstie, 2003d); results indicate that a coarsely discretized MINLP model can be used as a decision tool to provide useful design recommendations. Partial model validation versus temperature measurements positively attests to its reliability and encourages further investigation of its assumptions and predictive potential.

First Level: MINLP Voltage Optimization

The present study considers the MINLP model developed for electrode position and voltage optimization of the 2nd reactor stage (Gerogiorgis and Ydstie, 2003d) and critically reviews the accuracy of the macroscopic spatial decomposition simplification upon which it relies (similarly: Bermingham et al., 1998; Bezzo et al., 2000).

For the purpose of this coarse first-level MINLP model we consider a series of N steady-state CSTR finite volumes and a fixed maximum (N) of electrodes that can be installed at fixed locations along the horizontal ARP axis; the goal is to perform electrode voltage optimization under balance and operation constraints, for $Al_{(l)}$ maximization. Species concentrations are derived using an Arrhenius kinetic model that was proposed by Frank et al. (1989). The strong assumptions made regarding spatial structure consider sharp vertical splits between adjacent CSTRs, implying negligible horizontal backmixing phenomena. Figure 2 illustrates the electrode voltages and positions: evidently, Joule heating is most important as close to the inlet of the ARP reactor 2nd stage as possible (on the left).

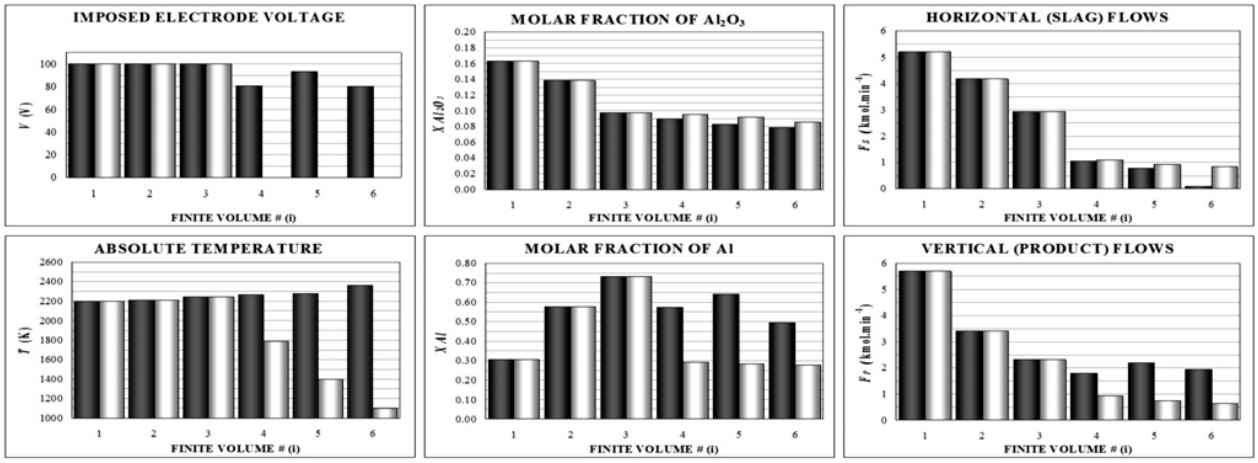

Figure 2: MINLP electrode voltage optimization for Al maximization: N=3 (gray columns) and N=6 (black columns).

Second Level: Two-Phase CFD Simulation

Direct multiphysics CFD simulation of the reactor has been undertaken as an essential part of advancing with the computer simulation goals pursued in collaboration with ALCOA and ELKEM for efficient ARP process R&D. Multiphysics CFD simulation of the reactive slag flow is also important as a tool for verifying the reliability of the aforementioned MINLP modeling assumptions and hence qualitatively examining the accuracy of MINLP results.

The CFD model is presented in the following section. The imposed voltages on electrode tips (V_i , i=1-6) are set, zero voltage (V = 0) is used on long horizontal sides to approximate the potential in the third (lateral) dimension, and zero gradient ($\nabla V = 0$) is used on all other wall sides. Inlet slag (2173 K) and wall (473 K) temperatures are set, and ideal insulation ($\nabla T = 0$) is assumed at electrode tips. An inlet hydrostatic pressure is assumed (P_0 = 200 Pa), with a no-slip boundary condition used on walls and tips for explicitly modeling $CO_{(g)}$ generation via Equation (7). A slip boundary condition is used for the slag free surface and zero pressure is assumed at the outlet (right end). Elimination of Lorentz (field) and Boussinesq (buoyancy) forces from the momentum balance of Equation (5) is based on the use of high-frequency AC electrodes and the negligible slag heat expansion coefficient (α), respectively. Figure 3 illustrates the slag velocity distribution under gas generation conditions, clearly indicating the development of well defined recirculation regions above each electrode.

Multiphase Flow CFD Model Equations

The steady state CFD problem considered comprises five PDE balances solved on a two-dimensional domain. The first part is the steady state electric charge balance:

$$\nabla^2 V = V_{xx} + V_{yy} = 0 \tag{1}$$

The second part is the steady state heat balance:

$$\nabla \cdot (k\nabla T - \rho C_P T\mathbf{U}) + \sigma(\nabla V)^2 - k_0 \exp\left(\frac{-\Delta G}{RT}\right)\Delta H = 0 \tag{2}$$

The third part is the steady state momentum balance:

$$\rho(\mathbf{U}\cdot\nabla\mathbf{U}) - \nabla\cdot\left[\left(\mu + \rho\frac{C_\mu}{\sigma_k}\frac{k^2}{\varepsilon}\right)\cdot\left(\nabla\mathbf{U} + (\nabla\mathbf{U})^T\right)\right] = -\nabla P \tag{3}$$

which also comprises the incompressible continuity PDE:

$$\nabla\cdot\mathbf{U} = 0 \tag{4}$$

complemented with the two standard k-ε model equations:

$$\rho(\mathbf{U}\cdot\nabla k) - \nabla\cdot\left[\left(\mu + \rho\frac{C_\mu}{\sigma_k}\frac{k^2}{\varepsilon}\right)\nabla k\right] = \rho C_\mu \frac{k^2}{\varepsilon}\left(\nabla\mathbf{U} + (\nabla\mathbf{U})^T\right)^2 - \rho\varepsilon \tag{5}$$

$$\rho(\mathbf{U}\cdot\nabla\varepsilon) - \nabla\cdot\left[\left(\mu + \rho\frac{C_\mu}{\sigma_\varepsilon}\frac{k^2}{\varepsilon}\right)\nabla\varepsilon\right] = \rho C_{\varepsilon 1} C_\mu k\left(\nabla\mathbf{U} + (\nabla\mathbf{U})^T\right)^2 - \rho C_{\varepsilon 2}\frac{\varepsilon^2}{k} \tag{6}$$

The two-phase flow is studied via a gas volume balance:

$$\nabla\cdot\left(\mathbf{D}R_b U_s(1-\varphi)\nabla\varphi - U_s\varphi(1-\varphi)\mathbf{e_g} + \varphi\mathbf{U}\right) = 0 \tag{7}$$

Our multiphysics CFD simulation results are discussed in an upcoming publication (Gerogiorgis and Ydstie, 2004).

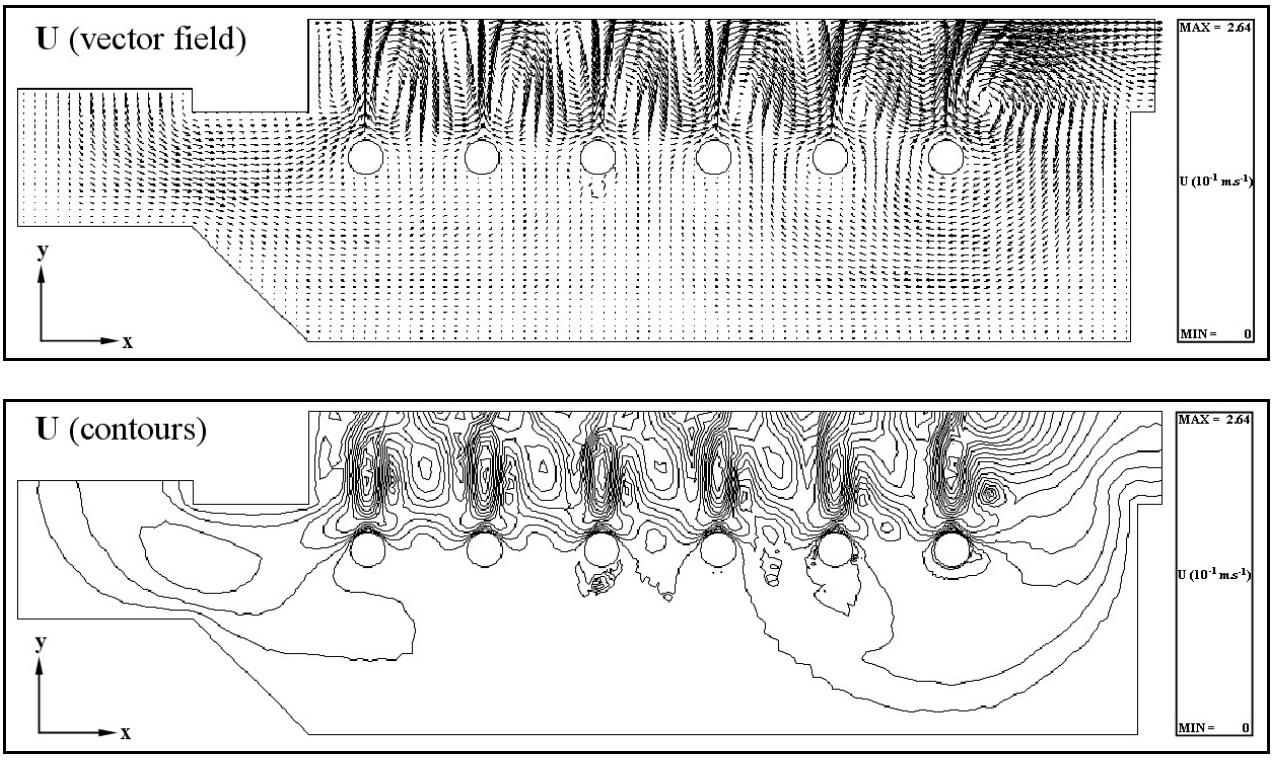

Figure 3: Direct multiphysics CFD simulation: vector field and contours of molten slag velocity under gas generation.

Conclusions

The two-level steady state multiscale process model previously proposed (Gerogiorgis and Ydstie, 2003a) has been analyzed with respect to the accuracy and reliability of the first-level MINLP electrode voltage optimization conducted for an one-dimensional two-phase discretization of the ARP carbothermic reactor 2nd stage using GAMS®. Direct second-level multiphysics CFD simulation has been employed in order to elucidate molten slag flow patterns under high-temperature intense gas generation conditions. The procedure entails the simultaneous solution of electric charge, heat, momentum, mass and gas fraction balances on a two-dimensional discretization using FEMLAB® 2.3; the slag velocity distribution is then evaluated against the fundamental assumptions previously stated made for the one-dimensional discretization made in the MINLP model. Explicit $CO_{(g)}$ generation modeling is quintessential here, as it has not been considered in previous papers and it is unclear if and how it affects MINLP model assumptions. Possible existence and intensity of horizontal backmixing phenomena is of importance here, because in that case the prior assumption of uniform downstream flow is violated and hence previous MINLP results are of limited accuracy. Relevant CFD and MINLP modeling details are published (Gerogiorgis and Ydstie, 2003c and 2003d, respectively). Conclusions are summarized in the following paragraphs.

The slag velocity vector field illustrated in Figure 3 clearly indicates a variety of remarkable characteristics: **(a)** the nearly quiescent slag flow under the electrode line, a result of the absence of observable gas production therein **(b)** the gradually increasing downstream vorticity above the electrode line, resulting in a remarkably strong vortex that is evident above and on the right of the last electrode: this vortex interacts with the adjacent reactor wall and produces a secondary, weak long-range recirculation flow. **(c)** the vertical slag entrainment flow above each electrode that is a result of intense $CO_{(g)}$ generation in these regions and reflects our constant slag/gas slip velocity assumption. The vertical recirculation features a well defined structure: individual recirculation regions are clearly disjoint, hence indicating that backmixing flow interactions are negligible and that MINLP assumptions do not violate flow profiles. Furthermore, the midpoints in between electrode pairs are confirmed as suitable vertical boundaries (MINLP model). The slag velocity contour field also illustrated in Figure 3 provides further evidence supporting the suitability of our assumptions: high-value velocity contours are densely and consistently concentrated above and close to all electrodes, confirming vertical splits as suitable in between electrodes.

The majority of prior MINLP modeling assumptions has thus been confirmed as reliable for design purposes. Horizontal slag backmixing is indeed negligible, with the notable exception of deep recirculation close to the outlet. Moreover, locally intense vertical gas flows suggest that the CSTR assumption is weak and more elaborate analyses can greatly improve the accuracy of composition estimates.

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