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Three-Dimensional Current Distributions in a Bipolar, Chlor-Alkali Membrane Cell

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The current distributions in a stack of bipolar, membrane chlor-alkali cells are important design considerations (1). The degree of nonuniformity of the current distribution is important to know because highly nonuniform current distributions could cause, among other things, severe damage to the membrane in a cell stack (2).

Recently, Dimpault-Darcy and White (3) used a computer program named TOPAZ2D (4), which is based on the finite element technique, to predict the two-dimensional current and potential distributions for bipolar plate electrolyzers. In that paper they stated that TOPAZ3D (5) could be used to predict current and potential distributions for three spatial coordinates, but they did not present any results.

The finite element method has also been used by others (6-12) to predict current and potential distributions in chlorine cells (6, 7), electroplating cells (8-10), and corrosion processes (11, 12). Morris and Smyrl (12) did use three spatial coordinates in some of their work, but they did not consider the spatial dependence of the specific conductivities, as done here. The purpose of this paper is to present the current distributions obtained by using TOPAZ3D for a three-dimensional section of bipolar, membrane chlor-alkali cell which includes portions that have spatial-dependent specific conductivities.

Figure 1 is a schematic of the section of a bipolar membrane cell (see Ref. (1) and (13) for a description of the cell) considered here. As shown in Fig. 1, a set current enters the anode from the boss portion of an anode/cathode element, passes through the various regions of the cell, and leaves through the boss portion of the next anode/cathode element. Only one quarter of a boss and the associated cell components are considered because of the symmetry of the components in the middle of the cell. Even though the results presented below do not apply to sections of the cell near the edge of the stack, the tech-
nique could be used to study those sections, if desired. The number and placement of the bosses (or gophers as they are sometimes called) affects significantly the current distribution in the cells; however, this is not considered in this paper.

It is not shown in Fig. 1, but the anodes and cathodes used in these cells are made of expanded metal. Consequently, the effective conductivity of each electrode depends on direction. This complexity was included in the model of the cell.

**Method**

Steady-state three-dimensional current and potential distributions in electrolysis cells can be predicted by using the heat transfer code called TOPAZ3D (5). The procedure for this consists of casting the charge transfer problem into a form suitable for solution by using the heat transfer program. This can be done by recognizing that charge is conserved in the region of interest and writing the appropriate equations to describe this. Charge will be conserved in a region if the divergence of the current density in that region is zero

$$\nabla \cdot i = 0 \text{ in } \Omega \tag{1}$$

where $i$ is given by Ohm's law.

$$i = i_x + i_y + i_z = - \left( \kappa_x \frac{\partial \Phi}{\partial x} + \kappa_y \frac{\partial \Phi}{\partial y} + \kappa_z \frac{\partial \Phi}{\partial z} \right) \tag{2}$$

Substitution of Eq. [2] into Eq. [1] yields the governing equation for the potential $\Phi$ at steady-state conditions

$$\frac{\partial}{\partial x} \left( \kappa_x \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \kappa_y \frac{\partial \Phi}{\partial y} \right) + \frac{\partial}{\partial z} \left( \kappa_z \frac{\partial \Phi}{\partial z} \right) = 0 \text{ in } \Omega \tag{3}$$

On a surface segment $\Gamma_1$ of the solid $\Omega$, it is assumed here that charge transfer can be represented by

$$\kappa_x \frac{\partial \Phi}{\partial x} n_x + \kappa_y \frac{\partial \Phi}{\partial y} n_y + \kappa_z \frac{\partial \Phi}{\partial z} n_z = i_{1,i} \text{ on } \Gamma_1 \tag{4}$$

where $i_{1,i}$ is the current density in $\text{A/cm}^2$ and is determined by dividing the set current that passes through $\Gamma_1$ by the projected area of that surface segment. Insulated surfaces (or surfaces of symmetry) are handled by setting $i_{1,i}$ equal to zero.

TOPAZ3D can be used to determine $\Phi(x, y, z)$ and then $i$ by using the dimensionless temperature option. This selection means that the dependent variable in TOPAZ3D must be dimensionless. Consequently, it is necessary to make $\Phi$ dimensionless. One way to do this is to define a reference potential $\Phi_{\text{ref}}$ and use it to make $\Phi$ dimensionless

$$\Phi = \Phi/\Phi_{\text{ref}} \tag{5}$$


$$\frac{\partial}{\partial x} \left( \kappa_x \frac{\Phi}{\Phi_{\text{ref}}} \right) + \frac{\partial}{\partial y} \left( \kappa_y \frac{\Phi}{\Phi_{\text{ref}}} \right) + \frac{\partial}{\partial z} \left( \kappa_z \frac{\Phi}{\Phi_{\text{ref}}} \right) = 0 \text{ in } \Omega \tag{6}$$

and

$$\kappa_x \frac{\partial \Phi}{\partial x} n_x + \kappa_y \frac{\partial \Phi}{\partial y} n_y + \kappa_z \frac{\partial \Phi}{\partial z} n_z = i_{1,i}/\Phi_{\text{ref}} \text{ on } \Gamma_1 \tag{4}$$

**Results and Discussion**

Values for $\Phi$ can be found by using TOPAZ3D after specifying the geometry and surfaces of the region $\Omega$ and selecting values for $\kappa_x, \kappa_y, \kappa_z, i_{1,i}$, and $\Phi_{\text{ref}}$. If the region $\Omega$ consists of several different parts, the values for the specific conductivities for each region must be specified. This can be done easily by utilizing INGRID (14) to prepare the finite element grid for all of the parts of the cell section shown in Fig. 1.

Figures 2 and 3 show the current distributions of the back side and front side of the anode, respectively, which were obtained by using input values appropriate for the cell segment shown in Fig. 1. For example, the anode considered here was of the expanded metal DSA type. To account for this in the model, values for the specific conductivities in the $x, y,$ and $z$ directions were set as follows: $\kappa_x = 1.03 \times 10^4 \text{ cm}^{-1}$, $\kappa_y = 1.26 \times 10^4 \text{ cm}^{-1}$, and $\kappa_z = 1.98 \times 10^3 \text{ cm}^{-1}$. The other input values used for the case presented here are available from the authors upon request. As can be seen by comparison of Fig. 2 and 3, the nonuniform current density distribution on the back side of the anode becomes relatively uniform on the front side. This is due to the highly conductive material used as the anode. Similar plots (not presented here) show that the current density distribution through the membrane is essentially uniform for this cell configuration and current.
density; and, consequently, should prevent overheating or blistering of the membrane and damage to the membrane due to nonuniform current distributions and impurities.

Summary

TOPAZ2D (5) can be used to determine current density distributions in electrolysis cells as demonstrated for a section of a bipolar, chlor-alkali membrane cell. The current density for the electrolysis cell considered here was about 0.62 A/cm². The resulting current density in a typical boss portion of the cell was about 25 A/cm². However, because of the high conductivity electrodes used in the cell, the current density distribution through the membrane portion of the cell was found to be essentially uniform.

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LIST OF SYMBOLS

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<th>Symbol</th>
<th>Description</th>
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<tr>
<td>i</td>
<td>current density vector, A/cm²</td>
</tr>
<tr>
<td>(i_n)</td>
<td>current density on surface segment i, A/cm²</td>
</tr>
<tr>
<td>(\eta_x, \eta_y, \eta_z)</td>
<td>dimensionless directional cosines</td>
</tr>
<tr>
<td>x, y, z</td>
<td>coordinates in cm</td>
</tr>
<tr>
<td>(\kappa_x, \kappa_y, \kappa_z)</td>
<td>specific conductivities, (\Omega^{-1} \text{ cm}^{-1})</td>
</tr>
<tr>
<td>(\Phi)</td>
<td>potential, V</td>
</tr>
<tr>
<td>(\Phi_{\text{ref}})</td>
<td>reference potential (\left(\Phi_{\text{ref}} = 1\text{V here}\right)), V</td>
</tr>
<tr>
<td>(\phi)</td>
<td>dimensionless potential</td>
</tr>
<tr>
<td>(\Omega)</td>
<td>region of interest</td>
</tr>
<tr>
<td>(\Gamma_i)</td>
<td>surface segment i on (\Omega)</td>
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Greek

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Predicted Secondary Current Distributions for Linear Kinetics in a Modified Three-Dimensional Hull Cell

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Current density distribution is an important consideration for those involved in designing electrochemical systems and electroplating systems in particular. Although it is important, the common practice in industry is to use trial and error to determine designs that optimize current density distributions in electroplating. The purpose of this paper is to illustrate the use of the finite element method (FEM) to predict three-dimensional current density distributions.

Two-dimensional FEM has been used successfully in modeling corrosion systems (1-8), electrolyzers (9), and three-phase cells (10, 11). Alkire, Bergh, and Sani (12) were among the first to apply the finite element method to electrochemical potential distribution problems. They studied the shape changes in electrodes during electrodeposition. The system studied was composed of a cathode made with parallel metal strips separated by an insulator and an anode at a fixed distance. Transient analysis using the FEM provided a time history of cathode shape during deposition. Finite element results agreed to within 2-5% of the analytical solutions. Micromechanics of multilayer printed wiring boards have also been studied using the FEM. Lee et al. (13) studied the thermomechanical strain in printed wiring boards. They constructed a finite element model for both plated through-holes and buried via structures to calculate the stresses in the copper barrel and at the via junctions.

An illustrative example of the use of the FEM in electroplating is given by Matlosz et al. (14). In their paper they compared the finite element solution to data obtained in a Hull cell to those obtained experimentally and through the boundary element method (BEM). The Hull cell is used commonly for visual measurement of the quality of electrochemical solutions (15). Most plating solutions are tested using a current of 2A and a plating time of 10 min (16). The slanted cathode used in this cell allows for a range of current densities, and how much of it is covered with deposit will depend on the quality of the solution.

TOPAZ2D (17) and TOPAZ3D (18) are finite element codes designed specifically for heat transfer problems. White et al. (19) used TOPAZ2D to predict current and potential distributions in a bipolar chlor-alkali membrane cell. They also present an example of the use of INGRID (20), a program that serves as preprocesser to TOPAZ3D. Topaz programs have a feature that most other finite ele-

REFERENCES