MASTER

PERFORMANCE MODEL FOR MOLTEN
CARBONATE FUEL CELLS

Quarterly Report for
5 July through 5 October 1978

D. Bloomfield, M. L. Finson, G. Wilemski,
T. Wolf and K. L. Wray

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ABSTRACT

Progress on the development of a performance model for molten carbonate fuel cells is reported. Key physical and chemical phenomena have been identified for inclusion in the model. In some instances, mathematical analyses of these phenomena have been begun. A numerical scheme to calculate the cell current density distribution has been developed. The scheme accounts for CO utilization and nonisothermal temperature distributions in the cell.

SUMMARY

This report is a description of work performed under U. S. Department of Energy Contract No. ET-78-C-03-2083 directed towards the development of a performance model for molten carbonate fuel cells. In this first quarter of the program we have concentrated mainly on determining the key physical and chemical phenomena to be included in the model.

In the differential cell model, which describes the local current density-voltage relationship at a point in the cell, attention must be paid to the mass transport of gaseous and dissolved reactants and products, to the ohmic resistance of electrolyte within the porous electrode, and to the electrokinetics taking place at the electrode surface. Tentatively, the thin film model of a porous electrode has been assumed as the basis for this investigation. While this phenomenological model is being developed, an empirical current-voltage relationship is being used in computational work associated with modeling of the integral cell.

Developments on the integral cell model have been directed towards the determination of the distribution of current density and temperature within the cell. The mass balance scheme needed for the calculation of the current density distribution in the cell has been devised. The scheme accounts for the utilization of CO_2 and O_2 in the cathode gas stream and of H_2 and CO , which are coupled by the water gas shift equilibrium, in the anode stream. By defining utilizations in terms of molar flow rates, the formulation can be applied without modification to nonisothermal cell conditions. A working computer code has been fashioned for the simpler case in which CO utilization is neglected.

Calculation of the cell temperature distribution depends on the treatment of heat transfer within the cell. Initially only the effects of gas phase transport of heat evolved in the electrode plane are being included. Conduction of heat in the plane of the cell through cell hardware will be

considered later. For now, then, all of the heat liberated in the cell is assumed to be transferred to the flowing gas streams either conductively or convectively by the flow of mass across the electrode/gas stream boundary arising from the cell half reactions. For the low Reynolds number flows typically found in anode and cathode streams, changes in fluid properties and the heat addition rate occur sufficiently slowly to justify the assumption of "locally fully developed" flow in which velocity and temperature relax instantaneously to fully developed profiles at each streamwise station. This approximation will entail an appreciably simplified analysis, yet it should provide the desired accuracy for electrode and gas stream temperatures.

I. INTRODUCTION

The objective of this program is the development of a molten carbonate fuel cell model that describes cell performance (current density versus voltage) as a function of inlet gas compositions, temperatures, flow rates and pressure. In addition, the model should provide a clear picture of the temperature and current density distributions over the electrode faces. The model can be conveniently discussed in terms of its three main components: a differential cell model (DCM) and two integral cell models, (ICM-I and ICM-II).

In the DCM, cell performance will be described on a local basis by incorporating phenomenological treatments of electrokinetics, mass transport, and porous electrode structure. The primary output of this model will be the current density as a function of local gas conditions, temperature and voltage. The other principal output of this model is the local heat release rate which is easily determined once the local current density is known.

The integral cell models treat cell behavior on an overall basis, accounting for fuel and oxidant utilization and heat transfer within the cell. In the ICM-I the output of the DCM will be combined with treatment of gas phase mass balance and convective heat transfer in order to calculate current density and temperature distributions in the cell. Heat conduction in the plane of the cell is not included in the ICM-I. This effect is incorporated in the ICM-II which is otherwise essentially identical with ICM-I.

II. DIFFERENTIAL CELL MODEL

A. Phenomenological Model

Our goal here is to give a phenomenological treatment of the local current density-voltage relationship in terms of molecular, kinetic and electrode parameters. Presently, it appears most fruitful to employ an idealized model of a porous electrode. In this analysis, the equations used to describe the kinetic and mass transport processes occurring must be solved for a set of boundary conditions consistent with an assumed pore geometry and electrolyte distribution. This kind of approach has been developed in the past by several groups of workers,^{1, 2, 3} and we will utilize their methods. Ideally, a more realistic theory of the porous structure of the electrode would be desirable but analyses starting from this premise have either provided very oversimplified treatments⁴ of kinetics and mass transport or are based on averaging processes^{5, 6} that leave fundamental mass transport and kinetic parameters difficult to interpret.

Estimates made of limiting current densities support the notion that extensive portions of the electrode surface must be covered by thin films of electrolyte.⁷ In Fig. 1, a sketch of the thin film model of an electrode pore is presented. The pore is taken to be a cylinder of radius R_p and is covered by a thin film of thickness δ for a length ℓ along the pore wall. The axial coordinate along the pore is z and r is the radial coordinate.

Fig. 1 Thin Film Model of an Electrode Pore

A simplified, but still mathematically complicated treatment of the mass transport and kinetics includes:

1. Diffusion of gaseous reactants and products into and out of the pore along the z axis; because we expect $R/l \ll 1$, we neglect radial gaseous diffusion.
2. Diffusion of dissolved reactants and products in the electrolyte along the r direction; we neglect z diffusion in the electrolyte because of the thinness of the film.
3. Use of Ohm's law to relate the change in overpotential η with z to the current I and ohmic resistance of the film.
4. Use of the Butler-Volmer equation to describe the transfer reaction kinetics.

Statements (1) and (2) imply that for each reactant (r) and product (p) we may write the equations

$$n_r F R_p D_{rg} \frac{d^2 c_{rg}}{dz^2} = 2i$$

$$n_p F R_p D_{pg} \frac{d^2 c_{pg}}{dz^2} = - 2i$$

$$n_r F r D_{rl} \frac{dc_{rl}}{dr} = - R_p i$$

$$n_p F r D_{pl} \frac{dc_{pl}}{dr} = R_p i$$

Here, D and c are a diffusion coefficient and molar concentration; the subscripts g and l label the gas and liquid phases, n is the number of moles of electrons transferred per mole of reactant or product, $I(z)$ is the total current in the film at z and i is the transfer current density:

$$\frac{dI}{dz} = 2\pi R_p i \quad (1)$$

Regarding statement (3), we may write for thin films¹

$$\frac{d\eta}{dz} = \frac{I(z)}{\kappa 2\pi R_p \delta} \quad (2)$$

where κ is the specific conductivity ($\text{ohm}^{-1} \text{cm}^{-1}$) of the electrolyte. Finally, the Butler-Volmer equation for the transfer current density has the general form:

$$i = i_o \left(\frac{\frac{c_{rl}}{0}}{\frac{0}{c_{rl}}} e^{\alpha \eta n F / RT} - \frac{\frac{c_{pl}}{0}}{\frac{0}{c_{pl}}} e^{-(1-\alpha) \eta n F / RT} \right) \quad (3)$$

for assumed first order forward and reverse reactions. Here, i_o is the exchange current density and α is the transfer coefficient. The superscript 0 denotes open circuit conditions, and the concentrations appearing in this expression are to be evaluated "at" the electrode surface just outside the compact double layer. The actual half reactions for the molten carbonate cell will more than likely not be first order in just a single reactant and product. A more complicated dependence is anticipated on the basis of past considerations.⁸ Thus, the Butler-Volmer equation will have to be adjusted to reflect the actual reaction mechanisms assumed to be occurring. This problem will be addressed in the next quarter when we will also begin examining the adequacy of the fits to IGT experimental small cell data⁸ with i - η relationships calculated from the above equations. We have not yet decided whether a full numerical solution of the above equations is needed or whether there

is sufficient separation of the physical regimes to allow satisfactory treatment from simpler (probably approximate) analytical solutions. As an example of the latter procedure, consider the following calculation.

At sufficiently low overpotentials (< 50 mV), the Butler-Volmer equation (Eq. (3) with $n=2$) can be linearized giving

$$i = \frac{2 i_o F}{RT} \eta \quad (4)$$

Under these conditions, it is likely that mass transport limitations will not arise, and we need only combine Eq. (1), (2) and (4) for the ohmic drop in the film to obtain

$$\frac{d^2 \eta}{dz^2} = \frac{i_o}{\kappa \delta} \frac{2F}{RT} \eta \quad (5)$$

The solution to this equation is

$$\eta(z) = \eta(0) \cosh(Kz) \quad (6)$$

where

$$K = \left(\frac{i_o 2F}{\kappa \delta RT} \right)^{1/2} \quad (7)$$

From Eq. (2) we also readily find

$$I(\ell) = 2 \pi R_p \delta \kappa K \tanh(K\ell) \eta(\ell) \quad (8)$$

Substituting the parameters listed in Table I into Eq. (7) we obtain a value of $K = 14 \text{ cm}^{-1}$. Equation (8) may be solved for the total pore overpotential in terms of the pore current. For an electrode current density of 100 mA/cm^2 and an electrode pore density $N_p = 4 \times 10^6 \text{ pores/cm}^2$ (Ref. (7)),

the pore current $I(\ell)$ is 25×10^{-6} mA/pore. Equation (8) yields a value of the pore overpotential $\eta(\ell) = 38$ mV. With this value of the overpotential at $z=\ell$, we may solve for the overpotential at the film end $z=0$ using Eq. (6). We find $\eta(0) = 30$ mV.

We may conclude from the above exercise that the 38 mV total pore overpotential justifies the linearization and that the resistive loss in the film is about 8 mV. Finally, the slope of the polarization curve ($N_p I(\ell)$ vs $\eta(\ell)$) is 2.6 mA/mV-cm^2 which is the same order of magnitude as that found in the experimental IGT data.⁸

TABLE I
(Based on values found in Ref. 7)

Parameter	Value
i_0	$4 \times 10^{-4} \text{ A/cm}^2$
κ	1 (ohm-cm)^{-1}
δ	$5 \times 10^{-5} \text{ cm}$
ℓ	$5 \times 10^{-2} \text{ cm}$
R_p	$2.5 \times 10^{-4} \text{ cm}$
T	923°K

B. Preliminary Empirical Model

In order to proceed with the development of a numerical scheme for predicting current density and temperature distributions in the cell (ICM-I) we have decided to employ a simplified analytical expression for the voltage drop V between electrodes as a function of local gas composition and pressure and local current density j :

$$V = E - jz_{\text{ohm}} - \eta \quad (9)$$

$$E = E^{\circ} - \frac{RT}{2F} \ln \left(\frac{X_{\text{H}_2\text{O}} X_{\text{CO}_2}}{X_{\text{H}_2}} \right)_A + \frac{RT}{2F} \ln \left(X_{\text{O}_2}^{1/2} X_{\text{CO}_2} \right)_C + \frac{RT}{4F} \ln P$$

Here, E is the open circuit potential at the local temperature T and gas conditions, X is the mole fraction in a gas stream, P is the gas pressure, and z_{ohm} is the ohmic impedance of the electrolyte. Finally, η is the sum of the electrode overpotentials which, for the present, we take as linear in the current density based on the experimental findings of IGT.⁸

The local heat release rate is given by the following equation (in units of watts/cm²):

$$\dot{q} = j(\Delta H/2F + V) \quad (10)$$

where ΔH is the enthalpy change for the overall cell reaction at the local temperature T . Because the anode and cathode temperatures are not likely to differ by more than a few degrees at any point in the cell, we are simply using an average cell temperature for each point in the electrode plane. We are also assuming that the electrodes are perfect electrical conductors and that ionic currents in the electrolyte are orthogonal to the electrodes. Eventually, all of these assumptions will be more critically examined, but for now they provide a physically sound basis for our modeling effort. Implementation of this preliminary DCM is discussed in the following section.

III. INTEGRAL CELL MODEL (I)

Our ultimate objective is the determination of current density and cell temperature distribution for a given set of operating conditions (cell voltage, inlet gas compositions and temperatures, pressure). For the ICM-I we have identified two reasonable computation schemes. The first of these is iterative in which a given temperature distribution is used to compute a distribution of current density, which is in turn used to update the temperature distribution, etc. An alternative is to proceed in a stepwise fashion, calculating the temperature and current density simultaneously at each point based on the upstream history of the gas flows. Which scheme is chosen will depend mainly on accuracy and speed of execution and on the anticipated ease with which in-plane heat conduction can be included at a later time.

Independent of the overall computational scheme selected, we can formulate the problem in terms of the performance of the two subtasks:

1. Calculation of the distribution of current density associated with a given temperature distribution.
2. Calculation of the temperature distribution associated with a given distribution of current density.

A. Current Density Distribution

1. Without CO Utilization

This calculation has previously been performed at IGT.⁸ Here we present a modification of that procedure and some preliminary results of our own. Our modification consists of redefining the anode and cathode conversions λ , μ in terms of molar flow rates rather than volume flow rates as in the IGT work:

$$\text{anode: } \lambda = \frac{\text{moles H}_2 \text{ consumed}}{\text{moles H}_2 \text{ in}} = \frac{\dot{n}_{\text{H}_2}^0 - \dot{n}_{\text{H}_2}}{\dot{n}_{\text{H}_2}^0}$$

$$\text{cathode: } \mu = \frac{\text{moles CO}_2 \text{ consumed}}{\text{moles CO}_2 \text{ in}} = \frac{\dot{n}_{\text{CO}_2}^0 - \dot{n}_{\text{CO}_2}}{\dot{n}_{\text{CO}_2}^0}$$

where $\dot{n}_i$ = molar flow rate of species i . Superscript 0 denotes an inlet quantity. This small change permits the variables λ and μ to provide an unambiguous measure of gas utilization even under nonisothermal conditions. Definitions involving volume flow rates suffer from the fact that volume flow rates change nonchemically because of expansion or contraction arising from temperature changes. The mathematical analysis needed to solve this problem under nonisothermal conditions also remains simpler when molar definitions are used. Of course, for isothermal conditions the two sets of definitions are equivalent. We also assume that the anode and cathode streams are constrained to flow in the cross flow direction (say by a network of parallel channels at each electrode). Denoting the anode flow direction as x , the cathode flow direction as y , and the channel width as w , requirement of conservation of mass leads to the equations

$$\frac{d\lambda}{dx} = \frac{1}{\dot{n}_{\text{H}_2}^0} \frac{jw}{2F} \quad (\text{anode}) \quad (11)$$

$$\frac{d\mu}{dy} = \frac{1}{\dot{n}_{\text{CO}_2}^0} \frac{jw}{2F} \quad (\text{cathode}) \quad (12)$$

applicable at each point on the electrode surfaces. As mentioned earlier we make the following additional assumptions:

1. The cell potential V is constant at all points in the cell.
2. The overpotential η is linear in current. We can then define a total effective impedance z_{tot} incorporating ohmic losses and electrode overpotentials.
3. The composition is uniform over the channel depth. This is approximately valid for sufficiently narrow channels, where species diffuse across the channel within a few channel widths downstream of their appearance at the electrode surface.

The mole fractions X_i in Eq. (9) can now be written in terms of conversions λ and μ . Solving Eq. (9) for current j , where we have substituted $\eta + jz_{\text{ohm}} = jz_{\text{tot}}$, gives

$$j(\lambda, \mu) = \left(E^0 + \frac{RT}{2F} \ln \left(\frac{K_c}{K_A} \right) + \frac{RT}{4F} \ln P - V \right) \frac{1}{z_{\text{tot}}} \quad (13)$$

where

$$K_A = \frac{\left(\dot{n}_{\text{H}_2\text{O}}^0 + \dot{n}_{\text{H}_2}^0 \lambda \right) \left(\dot{n}_{\text{CO}_2}^0 + \dot{n}_{\text{H}_2}^0 \lambda \right)}{\dot{n}_{\text{H}_2}^0 (1-\lambda)} \left(\frac{1}{\dot{n}_{\text{A}}^0 + \dot{n}_{\text{H}_2}^0 \lambda} \right)$$

$$K_c = \left(\dot{n}_{\text{O}_2}^0 - \frac{1}{2} \dot{n}_{\text{CO}_2}^0 \mu \right)^{1/2} \left(\dot{n}_{\text{CO}_2}^0 (1-\mu) \right) \left(\frac{1}{\dot{n}_{\text{c}}^0 - \frac{3}{2} \dot{n}_{\text{CO}_2}^0 \mu} \right)^{3/2}$$

Eqs. (11), (12) and (13) can be solved simultaneously for the unknowns j , λ , μ . A "marching forward" numerical integration scheme is appropriate, using

$$\lambda(x, y) = \frac{w}{2F\dot{n}_{H_2}^0} \int_0^x j dx'$$

$$\mu(x, y) = \frac{w}{2F\dot{n}_{CO_2}^0} \int_0^y j dy'$$

with the boundary conditions:

$$\lambda(0, y) = 0 \quad \mu(x, 0) = 0$$

We have so far written and debugged a computer code that computes the current density distribution from the above equations for a given cell temperature distribution. Results from an illustrative computation, carried out for an isothermal cell, are presented in Table III, for the following conditions:

TABLE II
CELL CONDITIONS FOR
CURRENT DENSITY DISTRIBUTION CALCULATION

	Anode Stream	Cathode Stream
Inlet Gas Composition	64% H ₂ , 10% H ₂ O 6% CO ₂ , 20% CO	20% CO ₂ , 20% O ₂ , 60% N ₂
Inlet Molar Flow Rates (moles/sec)	5 x 10 ⁻⁴	1.5 x 10 ⁻³
Cell Voltage = 0.75V, T = 920°K, P = 1 atm, z _{tot} = 1.025 ohm - cm ²		

TABLE III
ILLUSTRATIVE CURRENT DENSITY DISTRIBUTION

CURRENT DENSITY, AMP/CM**2									
0.331	0.301	0.281	0.266	0.254	0.243	0.234	0.225	0.218	0.211
0.329	0.300	0.280	0.265	0.252	0.242	0.233	0.224	0.217	0.210
0.327	0.298	0.279	0.264	0.251	0.241	0.232	0.223	0.216	0.209
0.325	0.297	0.277	0.262	0.250	0.240	0.230	0.222	0.215	0.208
0.323	0.295	0.275	0.261	0.249	0.238	0.229	0.221	0.214	0.207
0.320	0.293	0.274	0.259	0.247	0.237	0.228	0.220	0.213	0.206
0.318	0.291	0.272	0.258	0.246	0.236	0.227	0.219	0.212	0.205
0.315	0.288	0.270	0.256	0.244	0.234	0.226	0.218	0.211	0.204
0.312	0.286	0.268	0.254	0.243	0.233	0.224	0.217	0.210	0.203
0.308	0.283	0.265	0.252	0.241	0.231	0.223	0.215	0.208	0.202
LOCAL ANODE CONVERSIONS									
0.000	0.054	0.102	0.148	0.191	0.232	0.271	0.309	0.345	0.381
0.000	0.053	0.102	0.147	0.190	0.231	0.270	0.308	0.344	0.379
0.000	0.053	0.101	0.146	0.189	0.230	0.269	0.306	0.342	0.377
0.000	0.053	0.101	0.146	0.188	0.228	0.267	0.305	0.341	0.375
0.000	0.052	0.100	0.145	0.187	0.227	0.266	0.303	0.339	0.373
0.000	0.052	0.099	0.144	0.186	0.226	0.264	0.301	0.337	0.371
0.000	0.051	0.099	0.143	0.184	0.224	0.262	0.299	0.334	0.369
0.000	0.051	0.098	0.141	0.183	0.222	0.260	0.297	0.332	0.366
0.000	0.050	0.097	0.140	0.181	0.221	0.258	0.295	0.330	0.364
0.000	0.050	0.096	0.139	0.180	0.219	0.256	0.292	0.327	0.361
LOCAL CATHODE CONVERSIONS									
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.057	0.052	0.049	0.046	0.044	0.042	0.040	0.039	0.038	0.036
0.114	0.104	0.097	0.092	0.087	0.084	0.081	0.078	0.075	0.073
0.171	0.155	0.145	0.137	0.131	0.125	0.121	0.116	0.112	0.109
0.227	0.207	0.193	0.182	0.174	0.167	0.160	0.155	0.149	0.145
0.283	0.257	0.241	0.228	0.217	0.208	0.200	0.193	0.186	0.180
0.338	0.308	0.286	0.272	0.260	0.249	0.239	0.231	0.223	0.216
0.393	0.358	0.335	0.317	0.302	0.290	0.279	0.269	0.260	0.251
0.447	0.408	0.381	0.361	0.344	0.330	0.318	0.306	0.296	0.287
0.501	0.457	0.420	0.405	0.386	0.370	0.356	0.344	0.332	0.322

The current density is seen to be largest at anode and cathode inlet (331 mA/cm^2), where the gas streams are richest in fuel and oxidant content, and smallest at outlet (202 mA/cm^2) due to depletion of the gas streams. Note that current density falls off more sharply in the cathode flow direction along the anode inlet (7%) than along the anode outlet (4%), due to the tendency of the fresh anode gas to deplete the oxidant more readily than the partially utilized anode gas at outlet. The low utilizations for this case ($\lambda_{\text{avg}} = 37\%$, $\mu_{\text{avg}} = 39\%$) could be increased by reducing the gas flow rates, thereby boosting overall cell efficiency.

2. With CO Utilization

In order to account for the simultaneous utilization of CO and H₂ we note the following points. Under conditions typical of operating molten carbonate cells, direct electrochemical reaction of CO seems to be quite slow. On the other hand, water gas shift equilibrium

does seem to be preserved throughout the anode gas stream, probably via rapid heterogeneous reactions on exposed nickel anode surfaces. Thus CO utilization occurs indirectly via the shift reaction as H₂ is consumed electrochemically. Whether this sequence of events actually does occur is immaterial for the present calculation provided that the shift equilibrium is somehow maintained.

We use our earlier definition of H₂ utilization and provide a similar definition for the net CO utilization ρ :

$$\rho = (\dot{n}_{\text{CO}}^0 - \dot{n}_{\text{CO}}) / \dot{n}_{\text{CO}}^0$$

The total fuel utilization, on a molar basis, is the sum of λ and ρ .

Let ν be the fraction of current contributed by CO utilization. Then, from mass balance considerations, we find

$$\frac{d\dot{n}_{\text{CO}}}{dz} = - \frac{\nu j w}{2F} \quad \frac{d\dot{n}_{\text{H}_2}}{dz} = - \frac{(1-\nu) j w}{2F}$$

By adding these two equations together and substituting for $\dot{n}$ in terms of ρ and λ we obtain

$$\frac{2F}{w} \frac{d}{dz} (\dot{n}_{\text{CO}}^0 \rho + \dot{n}_{\text{H}_2}^0 \lambda) = j \quad (15)$$

This equation and the earlier equation for the oxidant utilization μ must be simultaneously integrated to determine ρ , λ and μ at all points on the electrode surface. As before, this integration requires knowledge of the dependence of j on the local gas composition and, hence, on ρ , λ and μ . In the remainder of this section we simplify the problem posed by Eq. (15) by relating ρ and λ through the water gas shift equilibrium.

For that equilibrium, in terms of mole fractions X , we have according to Eq. (14):

$$K_s = \frac{X_{H_2} X_{CO_2}}{X_{H_2O} X_{CO}} \quad (16)$$

From stoichiometric considerations we also have

$$\dot{n}_{H_2O} = \dot{n}_{H_2O}^0 + \lambda \dot{n}_{H_2}^0$$

and

$$\dot{n}_{CO_2} = \dot{n}_{CO_2}^0 + \lambda \dot{n}_{H_2}^0 + 2\rho \dot{n}_{CO}^0$$

Now we introduce the volume flow rate φ_A (cm^3/sec), the total (constant) pressure P , temperature T and gas constant R in the form

$$P\varphi_A x = \dot{n}RT$$

Then, the mole fractions X_i can be expressed as

$$X_{H_2} = \gamma(1-\lambda) X_{H_2}^0$$

$$X_{CO} = \gamma(1-\rho) X_{CO}^0$$

$$X_{H_2O} = \gamma \left(X_{H_2O}^0 + \lambda X_{H_2}^0 \right)$$

$$X_{CO_2} = \gamma \left(X_{CO_2}^0 + \lambda X_{H_2}^0 + 2\rho X_{CO}^0 \right) , \quad (17)$$

where

$$\gamma = \varphi_A^0 T \left(\varphi_A T^0 \right) .$$

When Eqs. (17) are substituted into Eq. (16), a little algebra produces

$$1-\rho = \frac{(1-\lambda) \left(1 + \lambda X_{H_2}^0 / X_{CO_2}^0 + 2X_{CO}^0 / X_{CO_2}^0 \right)}{\frac{K_s}{K_s^0} \left(1 + \lambda X_{H_2}^0 / X_{H_2O}^0 \right) + (1-\lambda) \left(2X_{CO}^0 / X_{CO_2}^0 \right)} \quad (18)$$

where K_s^0 is evaluated at the inlet temperature. Equation (18) can be used to eliminate ρ from Eq. (15), leaving it in a form suitable for integration.

In the very near future, we plan to determine current density distribution on the basis of Eqs. (6) and (15) in order to ascertain the effects of shift equilibrium on cell performance.

B. Temperature Distribution

The initial weeks of this effort have been spent identifying the predominant heat transfer mechanisms that occur in fuel cells, with particular attention given to modeling the heat transfer problem without undue complexity.

We assume that all of the heat $\dot{q}$ (see Eq. (10)) liberated in the cell is carried off by thermal convection in the gas streams, that the gas streams are constrained to flow in narrow channels, that the anode and cathode are locally at the same temperature, and that in-plane heat conduction can be neglected (for the present). Nevertheless, a precise calculation of the cell temperature remains a formidable task, due primarily to the following effects:

1. Gas composition and temperature, hence fluid properties, vary both across the depth of the channel and in the streamwise direction.
2. The mass and volume flow rates vary along the streamwise direction for each electrode.
3. The rate of heat addition varies along the streamwise direction.
4. Complex flow geometries are possible, e. g. baffling and channels of varying cross-section may be present.

Under these circumstances, a detailed calculation of the temperature profiles across the gas streams would require a finite-difference solution of the governing differential equations, involving significant computational complexity. Fortunately, we are only interested in the electrode temperatures and mean gas temperatures, which suggests the use of a "heat exchanger" type analysis. This offers considerable simplification, and can be expected to afford the desired degree of accuracy for the quantities of interest. This type of analysis is actually exact in the limiting case of constant property, fully developed flow with a constant rate of heat addition. For the present case of low Reynolds number flow, changes in fluid properties and the rate of heat addition occur sufficiently slowly to justify the assumption of "locally fully developed" flow in which velocity and temperature relax instantaneously to fully developed profiles at each streamwise station.

We must also account for heat fluxes associated with mass addition (anode) or subtraction (cathode) at the gas/electrode interface, as species entering or leaving the gas streams carry with them a characteristic enthalpy.

It is important to realize that the interface is taken to lie in infinitesimal distance inside the gas stream, so that the "electrode" encompasses the chemical reaction zone (gas phase reactions are presumed not to occur in the bulk stream). The model need not be sensitive to whether heat release/absorption occurs at the anode or cathode separately; because of sufficiently high tile thermal conductivity account is taken only of the total heat release per unit area evolved within the electrode-tile sandwich.

To summarize, if we neglect in-plane heat conduction, the local heat release at each point in the cell is transferred to the gas streams as a conductive flux by virtue of a temperature gradient at the gas/electrode interface, or as a convective flux due to mass transfer at the boundaries. The mathematical formulation of these concepts, the quantitative justification of our working assumptions, and the development of a computer code to implement them are scheduled to receive immediate attention in the next stage of our modeling efforts.

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