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CALCULATIONS OF TRANSPORT PHENOMENA IN SOLID-OXIDE FUEL CELLS

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ABSTRACT

This paper presents the results of a collaborative research project of computer modeling of transport phenomena within the passages of solid-oxide fuel cells. From a mechanical design viewpoint, fuel cells may be considered to be similar to heat exchangers with internal heat generation due to ohmic heating. This is a function of load-driven factors. The thermomechanical design of the units is of paramount importance, as the reaction rates are a function of temperature, pressure, and species concentrations, i.e., the process is fully coupled. The design goal of the project is to ensure uniform flow and temperature distribution throughout the stack, to optimize performance and minimize the risk of failure.

We developed computer models to predict the performance of cells and stacks of cells, so as to minimize the development of expensive experimental protypes and test rigs. The standard techniques of heat transfer and computational fluid dynamics were substantially modified to be applicable in this context. Three distinct approaches were considered. In all cases two fluids; air and fuel, each containing different chemical species were considered. The equations for fluid flow, heat and mass transfer with electro-chemical reactions occurring were discretized and solved using a finite-volume method. Detailed numerical simulations of a single cell and stacks of up to 54 cells were performed using fine three-dimensional meshes of up to 4.6 million cells. Simplified models based on a distributed resistance (porous media) analogy, and also traditional presumed flow methods used in heat exchanger and furnace design, were also employed. These latter approaches have the advantage of being readily executable on small personal computers. The three methodologies are described and compared in detail.

NOMENCLATURE

A	Area
b	Width
D	Mass transfer coefficient
F	Distributed resistance
F	Faraday's constant
Н	Height
h	Heat transfer coefficient
i	Local current density
J	Mass flux
k'	Inter-phase slip coefficient
L	Length of core assembly
Μ	Molecular weight
m	Mass flux
Ν	Number of cells in stack
p	Pressure
Ż	Volumetric discharge
<i>R</i> , <i>R</i> '	Lumped resistance
r	Volume fraction
S	Source term in finite-volume equations
t	Temperature
U	Overall area heat transfer coefficient
$ec{U}$	Superficial velocity
ū	Interstitial velocity
<i>u</i> , <i>v</i> , <i>w</i>	Velocity components
V	Cell voltage
x	Mole fraction
У	Mass fraction

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α	Volumetric heat transfer coefficient	
β	Conductance ratio	
Γ	Exchange coefficient	
γ	Volumetric mass transfer coefficient	
ν	Valence	
η	Overpotential	
μ	Viscosity	
ρ	Density	
φ	General scalar	
Subscripts		
a	Air	

е	Electrolyte
i	Interconnect
f	Fuel

INTRODUCTION

Fuel cells convert chemical energy into electrical energy and heat (Appleby and Foulkes, [1], Kordesh and Simader [2]). Fuel (hydrogen or methane) is fed into the anode of the cell, and oxygen or air, is supplied via the cathode. Oxygen ions are transported through the solid oxide electrolyte, reacting with hydrogen at the anode to form water. Electrons flowing through the external load provide a current. Solid oxide fuel cells (SOFC's) offer the advantage that methane or natural gas may used in the place of hydrogen, as fuel. The reaction is exothermic, operating at up to 1 000 °C.

Planar fuel cells are normally operated in stacks separated by interconnects. Figure 1 shows a group of four industrial SOFC stacks. The interconnects serve to pass the electrical current, and provide a pathway for reactants and products. Hydraulically, the cells are in parallel, with fuel and oxidant being supplied and removed via manifolds. The configuration is in some ways similar to a single-pass cross-flow heat exchanger. Figure 2 illustrates the flow pattern. For the fuelside both planar and rectangular ducts were considered, while for the air-side, only the former were considered. Heat management is a matter for concern: If the cell temperature is too low the chemical reaction will shutdown, while if it is too high, mechanical failure of the system may occur: Since cells are connected in series electrically; if one cell fails, the entire stack is rendered useless. It is thus very important that the supply of air and fuel, and the reaction rates in the cells be such that the temperature distribution is reasonably uniform. Air and fuel are continuously being depleted in the cell passages as a result of the chemical reaction(s); in this study source and sink terms due to chemistry, and associated mass transfer analysis are accounted for in a limited fashion, in addition to fluid flow and heat transfer.



Figure 1. Four fuel cell stacks connected to a common manifold. (From Global Thermoelectric Inc., with permission.)

The development of numerical models gives insight into the extent to which non-uniformities in flow distribution and heat transfer are acceptable, and provides an indispensable tool in dimensioning fuel cell stacks, minimizing the need for expensive test rigs at this pre-competitive stage of development. A fuel cell model for a single multi-plate cell assembly, and also manifold and stack models were therefore developed. Further details are provided below.

Literature review

Modeling of SOFC's can be traced to the early work of Archer and Sverdrup [3] and Sverdrup et al. [4]. Since then, various models have been developed and applied at different scales. Wepfer and Woolsey [5] incorporated transport and kinetic properties to model irreversibility as voltage losses in an electrical network. Dunbar et al. [6] conducted explicit modeling of transport and kinetic processes in SOFC's. Achenbach [7] developed a three-dimensional (3-D) stack model for SOFCs, including the kinetics of the reforming Bessette and Wepfer [8] developed a model to reaction. evaluate the current flow distribution and irreversibility in a stack, with the thermal field evaluated using a simple conduction model. Foster [9] employed a finite element analysis package to calculate the fluid flow and heat transfer in a tubular SOFC. Yakabe et al. [10] developed a 3-D single-unit model to simulate the fluid flow, heat transfer, electric potential and current density, and the internal stresses in a single-cell stack with double channels of co-flow and counter-flow pattern.

PROBLEM CONSIDERED







Figure 3. Type 2 (rectangular-duct) configuration, air side only.

We considered both single cells and stacks of 54 fuel cells. using three different mathematical models described below. The fuel passages were plane ducts while both rectangular and plane duct passages were considered on the air side. Figures 2 and 3 illustrate the geometry and notation used below. These are referred to as Type 1 and Type 2 cells, respectively.

GOVERNING EQUATIONS

Three approaches were considered in analyzing SOFC's; detailed numerical simulation, distributed resistance (porous media) analogy, and traditional heat/mass transfer analysis based on the assumption of quasi-uniform flow.

Detailed numerical simulation

While it was once true that computer memory and speed limitations prevented all but the smallest problems from being solved directly, this is not true today. In this research project both single cells and stacks of up 54 cells were modeled using this approach. Figure 4 shows the topology for the latter case.



Figure 4. SOFC stack prototype

Detailed numerical simulations involve computing the entire flow field using the complete set of transport equations,

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \vec{u}) = S \tag{1}$$

$$\frac{\partial(\rho \vec{u})}{\partial t} + \operatorname{div}(\rho \vec{u}; \vec{u}) = -\operatorname{grad} p + \operatorname{div} \mu \operatorname{grad} \vec{u}$$
(2)

$$\frac{\partial(\rho\phi)}{\partial t} + \operatorname{div}(\rho \bar{u}\phi) = \operatorname{div}\Gamma\operatorname{grad}\phi + S$$
(3)

where ϕ is a general scalar corresponding to enthalpy, mass fraction etc. Although only a single source, *S*, is shown, in practice there may be several. The equations may be discretized and solved using a finite-volume method Patankar [11]. The computational fluid dynamics code PHOENICS was employed for this purpose. A rectilinear mesh was passed through both solid (electrolyte and interconnect) and fluid (air and fuel) regions with material properties being set appropriately. The grid was not uniform, but was concentrated in the near-wall boundary layers for the manifolds and cells.

The source term due to Ohmic heating is treated both as a constant value, and also as a variable to be computed iteratively. For the latter case electrochemical reactions are assumed to occur at the surface of the electrodes with source terms per unit area J (kg/m²s) (for H₂, H₂O and O₂) related to current density, *i* (A/m²), according to Faraday's law;

$$J = \pm \frac{Mi}{1000\nu F} \tag{4}$$

If the current density is considered variable, the cell voltage, V, may be expressed as,

$$V = E - iR - \eta_a - \eta_c = E - iR'$$
⁽⁵⁾

where η_a and η_c are anodic and cathodic overpotentials, and *R* is a local lumped resistance (Ωm^2). The open-circuit voltage or Nernst potential, *E*, is obtained as

$$E = E^{0} + \frac{RT}{2F} \ln \left(\frac{x_{H_{2}} x_{O_{2}}^{0.5}}{x_{H_{2}O}} \right) + \frac{RT}{4F} \ln p_{a}$$
(6)

The volumetric heat source (J/m^3s) in the electrolyte due to the combined effects of Ohmic heating and overpotentials may thus be written,

$$S = \frac{i(E-V)}{H_e} \tag{7}$$

A semi-empirical correlation, Ghosh et al. [12], Dong et al. [13] was used to compute R'. The calculation proceeds as follows: (1) Initial values are assumed for transport properties, cell voltage V etc. (2) Heat and mass source terms are computed from Faraday's law. The transport equations are then solved. (3) The open circuit voltage and internal resistance are then calculated, and the local current density obtained. Steps (2) and (3) are repeated until sufficient convergence is obtained.

Distributed resistance analogy

The method here is a modified version of the distributed resistance analogy of Patankar and Spalding [14], Spalding [15]. Beale et al. [16] employed this methodology considering the flow of a single phase (only) in the manifolds and passages of a SOFC in the absence of heat and mass transfer. Here simultaneous flow of both working fluids with the associated coupled heat/mass transfer is computed using local volume averaging so that,

$$\frac{\partial (r\rho)_k}{\partial t} + \operatorname{div}(r\rho\vec{u})_k = S_k \tag{8}$$

$$\frac{\partial (\rho r \vec{u})_k}{\partial t} + \operatorname{div} (\rho r \vec{u}; \vec{u})_k = -r_k \operatorname{grad} p_k - F_k r_k^2 \vec{u}_k$$
(9)

$$\frac{\partial \left(\rho c_p r t\right)_k}{\partial t} + \operatorname{div}\left(r \rho \vec{u} t\right)_k = \overline{\alpha} \left(t_e - t_k\right)$$
(10)

$$\frac{\partial (\rho r y)_k}{\partial t} + \operatorname{div}(r \rho \vec{u} y)_k = S_k$$
(11)

where k = a (air), f (fuel) or solid as appropriate. The temperature distribution in the electrolyte is also solved in the usual fashion. Because local volume averaging is employed, there are now two velocities and pressures p_a and p_r , corresponding to the air and fuel, in each computational cell, and temperatures in both fluid and solid regions. The chosen solution was to implement the multiply-shared space (MUSES) method in the PHOENICS code. The main ideas are to provide as many blocks of grid as necessary to cover the same volume of space in question and on each of these to solve for a different variable: (1) air; (2) fuel, (3) electrolyte, etc. Since values of variables (such as temperature) on any one grid may depend on those in another grid; these inter-phase terms are taken as sources.

In the momentum equations, the independent variable is the interstitial velocity $\phi = \vec{u}$, but the convection term is the superficial velocity $\vec{U} = r\vec{u}$. The viscous term is replaced by a resistance or drag distributed throughout the volume of the device. (NB. for negligible inertial effects $\vec{\nabla}p = -F\vec{U}$). For many fully-developed laminar duct flows, f = a/Re (based on hydraulic diameter, D_h). Under these circumstances it can be shown that $F = 2a\mu/rD_h^2$.

In the energy equation, the diffusion term is supplanted by an inter-phase term $\alpha(\phi_e - \phi_k)$, where α is a 'volumetric heat/mass transfer' coefficient. Similarly mass transfer is as above but per unit volume. Thus the distributed resistance method replaces diffusive effects with a rate equation (drag term), but inertial effects are still accounted for. It thus represents a model intermediate between direct numerical calculations and classical heat/mass transfer methods.

Presumed flow methods



Figure 5. Resistance diagram for heat transfer.

Traditional 'presumed flow' methods, based on a rate equation (heat/mass transfer coefficient), represent the simplest possible methodology. For constant velocity one may write,

$$\left(\dot{m}c_{p}\right)_{a}\frac{dt_{a}}{dx}=\beta_{a}\dot{q}+\overline{\alpha}\left(t_{f}-t_{a}\right)$$
(12)

$$\left(\dot{m}c_{p}\right)_{f}\frac{dt_{f}}{dy} = \beta_{f}\dot{q} + \overline{\alpha}\left(t_{a} - t_{f}\right)$$
(13)

where $\overline{\alpha} = U/H$ is obtained from the resistance diagram, Fig. 5, and β_a and β_f are conductance ratios e.g., $\beta_a = (UA)_{ae}/((UA)_{ae} + (UA)_{fe})$. Unlike above, it is here assumed that conduction in the electrolyte and interconnects is negligible so that $t_e = (\dot{q} + \alpha_{ae}t_a + \alpha_{fe}t_f)/(\alpha_{ae} + \alpha_{fe})$.



Figure 6. Temperature distribution in a Type 1 SOFC, constant heat source.



Figure 7. Temperature distribution in a Type 2 SOFC, constant heat source.



Figure 8. Temperature distribution in a Type 2 SOFC, heat source computed according to Eq. (7).



Figure 9. Pressure distribution in a SOFC stack, distributed resistance analogy.



Figure 10. Temperature distribution in a Type 2 SOFC stack, vertical plane.



Figure 11. Temperature distribution in a Type 2 SOFC stack, horizontal plane.

For constant heating it is thus possible to obtain a noniterative solution of the form,

$$t_{aP} = a_a + b_a t_{aW} + c_a t_{fS} \tag{14}$$

$$t_{fP} = a_f + b_f \phi_{aW} + c_f \phi_{fS} \tag{15}$$

where W= west of P, and S = south of P. However, if the source term is computed using Eq. (7), some iteration is required. Similarly for mass transfer,

$$\dot{m}(y_P - y_W) = \pm SV = \pm JA \tag{16}$$

Under these circumstances it is necessary to adjust the mass flow rates to account for the generation/depletion of matter due to electrochemical reactions, e.g., $\dot{m}_p = \dot{m}_W \pm SV$ on a volumetric basis. This is straightforward. A rate equation to compute the wall mass fraction from the source term, $S = \gamma (y_p - y_{wall})$ is used to the molar fractions in the Nernst equation, Eq. (6), and hence the Ohmic source term. The volumetric mass transfer coefficient is obtained from an appropriate Sherwood number correlation for the geometry.

RESULTS AND DISCUSSION

The results are summarized in Figs. 6 to 11 inclusive. Figures 6 and 7 show the temperature distribution in single Type 1 and 2 SOFC's for a constant heat source, corresponding to typical average operating conditions for the designs. Figure 8 shows the distribution in a Type 2 cell with the source term computed according to Eq. (7). For constant heat source, the temperature increases in a bilinear manner, as might be anticipated for a Neumann problem. However because the thermal capacitance of the oxidant is much larger than that of the fuel, the isotherms are more normally oriented across the ydirection. The temperature in the bulk of both working fluids is close to, but slightly lower than the temperature in the solid electrolyte, as is to be expected. Even for perfectly uniform heating, a significant temperature variation is inevitable across the cell unit. Departures from this behavior are due to the variation in heat source terms. Quantitative comparison of Figs. 7 and 8 is not appropriate, since the source term in Fig. 8 is a function of local concentrations, and temperatures and therefore not identical to Fig. 7, i.e., total current and current (power) density are computed iteratively, and not prescibed a priori in the latter case. However inspection of the local temperature variations indicates that the influence of variation of the temperature due to current density is not enormous. Power and current distributions may be found in Dong et al. [13]. Inspection of Eqs. (12)-(13) reveals that it is the ratio of the heat transfer coefficients, β , which is important if the correct fraction of heat generated is to be transferred to the appropriate working fluid. The 2-D temperature distribution is then a function of the capacitance ratio $(mc_P)_{min}/(mc_P)_{max}$.

Fig. 9 shows the pressure distribution in a Type 1 SOFC stack obtained from a distributed resistance analogy. The three spaces shown represent two fluid, and solid regions. It can be

seen that the pressure distribution in both fluids is quite uniform throughout stack in spite of flow variations in the inlet manifolds (not shown). This is because, as discussed in Beale et al. [16], if pressure losses across the manifolds are small compared to those across the stack, the flow and pressure distributions will be quite uniform within the core of the stack. As can be seen from the diagram, the MUSES method breaks up the interpenetrating continua into three (or more) domains facilitating graphical analysis readily.

Figures 10-11 show the temperature distributions in a Type 2 stack: The horizontal and vertical planes have been chosen at central locations within the body of the stack, Fig. 4. Variations in the vertical direction (i.e. 3-D) effects are illustrated in Fig. 10, and are more pronounced in the lower region of the stack. Although these will have an impact on reaction rates, they are however less significant than the primary gradients in the stream-wise plane which, as already discussed are always present due to Ohmic heating, regardless of the spatial distribution of the local current density. The zig-zag fluctuations in temperature are due to the presence of the small air ducts running across the flow, see Fig. 3. These are only apparent in detailed numerical simulations; local volume averaging removes these perturbations entirely. It is readily apparent that the temperature distribution in the horizontal stack plane is consistent with the single-cell results.

Because the flow is laminar; detailed numerical simulations can be relied upon to produce very accurate predictions of the performance of SOFC's. However the computational overhead is very large. The results presented here required meshes of over 4 million cells requiring more than 48 hours on a 32 processor PC beowulf. While in the future such calculations may be routine, at present these computational resources are significant by any standards, i.e. they could not be entertained on a day-today operation by fuel cell engineers not familiar in computational fluid dynamics. Moreover visualizing and analyzing the results of these data sets is far from easy due to the multiplicity of intermingling continua; display and manipulation of pressure and velocity data is far from easy.

Distributed resistance methods still require significant compute times, though not the same magnitude as are required for detailed simulations. It is true that some of the finer details are inevitably lost, however the approach allows for a reasonably accurate solution to be obtained in a reasonably short time. An advantage of the technique used in this paper is that diffusive effects may be included/excluded in different zones, so that a rate equation can be used selectively in certain regions, such as the stack core, but not in other regions such as manifolds and solids, see Fig. 4, where viscous and conduction terms are computed directly. The technique also allows for as many inter-phase terms (fluid-fluid, fluid-wall) etc. to be introduced as required, so that if, say, metallic conduction is insignificant this 'phase' may be removed.

Simple presumed-flow models provide a reasonable estimate for situations where the flow is known to be constant;

they should not be used for the design (sizing) of fuel cells, but may be used for analysis (rating), if it is known that cell has been properly designed, for uniform flow, in the first place. The main advantage of these methods is the near instantaneous compute times. Presumed flow methods are useful in certain situations, for example for control purposes or for investigating variation of parameters such as fuel/oxidant mass fractions, where a fast response is required.

There is of course no reason why the 'presumed' flow need be constant: Indeed it was not treated so here since mass sources due to chemical reactions were introduced on a cell-by-cell basis; Boermsa and Sammes [17] contains a simple lumpedcapacity hydraulic network appropriate for suitable modication for a continuum (i.e. resistance per unit volume) approach to compute pressure losses in the manifolds and stack assuming,

$\vec{\nabla} p = -F\vec{U}$, where $F = F_{\text{manifold}}$, F_{stack} etc.

The typical assumptions in conventional heat exchanger analysis [18] include steady-state operation, position independent heat/mass transfer coefficient, negligible losses to the environment, negligible metallic conduction etc. Many of these can still be relaxed in the simplified presumed-flow numerical integration scheme, provided some iteration is acceptable.

In both distributed resistance and presumed-flow methods, the overall heat transfer coefficients as well as the wall mass fractions are computed from an appropriate Nusselt/Sherwood number correlation. Thus the reliability of the calculations will depend on the efficacy of the appropriate correlations. In this study we used values [19] appropriate for constant flux (Neumann), rather than constant value (Dirichlet), however neither of these are strictly correct. Alternatively these may be obtained from experimental or detailed numerical analyses for the same design. Most of the correction factors used in heat exchanger design such as directional (not cross-flow), entrylength, wall (bypass) effects etc. are of minimal importance here.

Use of the Nernst equation should be considered, at best a loose approximation of reality, based as it is upon equilibrium thermodynamics, and is not valid when the utilization of fuel and/or oxidant is high. Moreover the assumption that the lumped resistance is a function of temperature only [12,13], is somewhat simplistic, however it is convenient for a first analysis.

The distributed resistance analogy [14] was originally developed to model transport phenomena in shell-and-tube heat exchangers, where there are substantial variations in the gross motion due to the presence of baffles. For the equipment under consideration; because the passages are straight and narrow, the flow is essentially uniform (notwithstanding mass sources/sinks due to the chemical reactions). Thus the computational overhead associated with the distributed resistance analogy is barely justified; since inertial effects are very small for the particular geometry under consideration. Coupling the presumed-flow heat/mass transfer solution for the fuel-cell stack to a flow solution for the manifolds etc. would appear to offer all the advantages of the distributed resistance analogy approach, with potential benefits in terms of speed of convergence, discussed below.

Convergence

A detailed simulation of a 54 cell stack with a 172x43x503 mesh required 48 hours to reach a converged solution. A distributed resistance analogy method with a 10x10x19 mesh took approximately 20 mins to obtain convergence.

In the latter context, Spalding [15] has discussed the need to employ a partial elimination algorithm when highly conductive zones connect the working fluids, as is the case here. Because the zones were coupled using simple source terms, i.e. a partial elimination algorithm was not implemented, there was a corresponding penalty in terms of speed-of-convergence. This was apparently aggrevated by the fact that the flow solver can not readily be aligned with main flow directions of both working fluids. The reader will note that in the simplified model, the cross-terms present in Eqs. (12) and (13) are algebraically eliminated in Eq.(14) and (15). Thus for the presumed flow code, convergence was near instantaneous, even when using meshes of the order 100x100, only 10 iterations per cell were required to compute the local curent density and heat and mass source terms.

CONCLUSIONS

Three classes of fuel cell model were developed in the source code and using existing computational fluid dynamics codes. 'Presumed flow' methods based on numerical integration using traditional heat/mass transfer rate equations provide simple 2-D results which, while of more than academic interest, are limited in their scope of application. Distributed-resistance analogy methods employing multiply-shared spaces, allow for inertial effects in 3-D flows to be accounted for, but require significantly more compute power. Detailed numerical solutions of the governing transport equations provide the best models for transport phenomena in solid-oxide fuel-cells, but the required computational requirements are close to the limits currently available.

The temperature distributions in solid-oxide fuel cells are dominated by the source terms (convection-source equations). Thus, a significant bilinear increase in temperature is observed, even when the current density is perfectly uniform. If this increase is sufficiently large to be of concern to the designer, Ohmic heating must be reduced by using materials with appropriately small electrical mobility. For the designs under consideration these gradients are close to the current design requirements. Local variations in lumped resistance and current density, while important, appear to be subordinate to the overall source term in the energy equations. However local temperature does influence reaction rates and mass transfer and air/fuel utilizability and hence should therefore be considered when developing detailed models.

In view of the current interest, design of fuel cells is proceeding in tandem with the development of new computational-based models, providing a new paradigm for engineering design.

FUTURE RESEARCH

The current work is research in progress. We are presently consolidating these preliminary results. Following this, we shall improve the diffusion models to incorporate Stefan-Maxwell equations for diffusion coefficients, thermal radiation effects and introduce additional chemistry to account both for internal reforming and water-shift reactions. Experimental data needed to validate models are being gathered and will be recorded in due course.

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