IN-44

DOE/NASA/0017-5
NASA CR-182188

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August 1988

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Printed in the United States of America

Available from
    National Technical Information Service
    U.S. Department of Commerce
    5285 Port Royal Road
    Springfield, VA 22161

NTIS price codes[1]
    Printed copy: A02
    Microfiche copy: A01

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MATHEMATICAL MODELING OF SOLID OXIDE FUEL CELLS

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Development of predictive techniques, with regard to cell behavior, under various operating conditions is needed to improve cell performance, increase energy density, reduce manufacturing cost, and to broaden utilization of various fuels. Such technology would be especially beneficial for the solid oxide fuel cell (SOFC) at its early demonstration stage.

Three designs of SOFC cell/stack configurations are now available and they are Westinghouse tubular, Argonne National Laboratory (ANL) monolithic, and Ztek planar FC models. A comparison among these designs in the previously stated areas is needed. Basically, the differences among these configurations are shape of cell, channel geometry for reactant flow, and size/thickness of cell components. These designs were compromised with manufacturability, which is still the most difficult task aspect of the SOFC development. Due to this difficulty, there are limitations on the size of monolithic and planar cells and on the weight (and cost) of tubular cell. But the manufacturability is not the only factor that limits the size of SOFC. As soon as the cell is put on operation, the temperature and the current density (CD) distributions on the plate will determine the success of the performance in the following ways: (1) hot spot temperatures exceeding the sintering, coating, or E(C)VD temperature will cause material problems, (2) severe non-uniform temperature distributions will result in cracking due to thermal stresses, and (3) non-uniform CD distribution will increase the possibility of reactant depletion at exit, especially at high utilization ratios. This paper describes the development of computer models to calculate the temperature, CD, and reactant distributions in the tubular and monolithic SOFCs. Results indicate that problems of non-uniform heat generation and fuel gas depletion in the tubular cell module, and of size limitations in the monolithic (MOD 0) design may be encountered during FC operation.

V-I Characteristics

The SOFC semi-empirical V-I characteristics was modeled with respect to cell components (thickness) and operating conditions (temperature, pressure, inlet fuel gas

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compositions, and fuel and oxidant utilization ratios).

Tubular Cell

For the Westinghouse tubular SOFC, a two-dimensional CD profile (circumferential and axial) was generated by assuming an isothermal condition (1000 °C). Recently reported performances of tubular SOFC using DOE specified fuel (67% H_2, 22% CO, 11 % H_2O at 85 % fuel utilization) and air [1] were applied in this study. First, an analytic model (Figure 1) was solved and the solutions were used to calculate the circumferential CD distribution around the tubular SOFC using specific fuel and oxidant gas flow rates. Because of symmetry, only one half of a cell was modeled. Secondly, a finite difference model was used to calculate the fuel and oxidant gas flow rates along the axis of the tubular SOFC. Reforming and water shift reactions were considered at equilibrium at the operating temperature of 1000 °C. Rated operating conditions and cell dimensions of the Westinghouse 5 kW module were applied. Figure 2 shows the circumferential and axial CD profiles. It is noted that there is non-uniformity of CD along the axis and around the circumference of the tubular cell. For a 0.275 A/cm^2 (average) operation, the CD ranges from 0.652 to 0.164 A/cm^2. The peak CD occurs at circumference equal to 1.85 cm in Figure 1, where the current flows radially out of the cell, and where the fuel and oxidant gases enter the cell axially. The lowest CD occurs at the opposite end of the cell. Figure 2 also shows that in an operating cell, the peak CD, as well as the largest heat generation, is near the interconnection. This will worsen the critical stress problem since the thermal expansion will not be compatible between the interconnection and other cell components.

Another important issue pertains to the probability of fuel gas depletion in the Westinghouse 5 kW module. The non-uniform fuel gas flow distribution in the passages (main, side, and corner) caused by the equal pressure gradient of the flow, is compared with the amount of fuel needed to achieve a parallel connection (e.g., the current for three cells in parallel is equal to 80 A). Documented performances from specimen testing [1] were adapted as the basis. Among these reported data, the performance is a function of the cell itself and the testing time. The probabilities of total fuel gas depletion (at operating time equal to 200 hours) around the edge cells for two types of flow passages and two to six cells in parallel are shown in Figure 3. It shows that in a design with three cells in parallel there is a 7% probability that fuel gas will be depleted at the exit of edge cells (corner cells and side cells in Type I & II flow distributions, respectively). In addition, a shorted cell (by assuming voltage of

arbitrarily chosen cell equal to 0) in the operation will always result in fuel gas starvation for the remaining, i.e., unshorted cells.

These results strongly imply that the design of more uniform fuel gas passages is necessary, which can be achieved by increasing the thickness of Ni felt or by redesigning the fuel gas intake plenum.

Monolithic Cell

Monolithic solid oxide fuel cells are currently being developed at Argonne National Laboratory. For many applications, operating conditions such as total pressure, average cell temperature and current density, as well as inlet reactant gas temperatures and compositions are fixed or are predetermined. A two dimensional computer model has been implemented to predict the effects of fuel utilization ratios (FUR), oxidant utilization ratios (OUR), and cell dimensions upon the temperature and current density distributions within cross-flow arrays of the MOD 0 design, subject to a specific set of the above mentioned operating conditions. Results from the model were used to determine limits on cell sizes and on reactant gas utilizations by evaluating the three performance indicators outlined earlier. In the subsequent analyses, the following operational parameters were maintained : pressure = 1 atm; average array temperature = 1000 °C; average current density = 500 mA/cm^2; inlet molar fuel gas composition : 97% H$_2$, 3% H$_2$O; inlet molar oxidant gas composition : 21% O$_2$, 79% N$_2$; and each inlet gas temperature = 800 °C.

All V-I relationships for the monolithic fuel cells were assumed to behave linearly within the range of interest. Some representative V-I curves are displayed in Figure 4, where the best case accounts only for ohmic resistance and the estimated case includes slow polarization effects. Both the best case and the estimated case are more favorable than the experimental V-I curve, however, it is reasonable to expect that the experimental relationship has been improved since the December 1985 status [2].

Figure 5 shows the relationship between FUR and OUR that must exist in order to satisfy the specified operating conditions. While Figure 5 represents the case for a 10 cm x 10 cm array, the shape of the curve is similar for other cell dimensions as well. It is evident from the figure that lower limits on both FUR and OUR will be encountered. The effect of FUR on overall operating efficiency is also depicted in Figure 5 and it is seen that the maximum efficiency is obtained at a relatively small FUR value, near FUR = 0.2 .

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A typical temperature distribution is shown in Figure 6 where the peak temperature is reached at the extreme corner of the array, since reactant gas depletion is at the maximum there. The minimum array temperature occurs at the opposite corner. In all cases, the maximum temperature is located along the edge of the array where oxidant gas departs, however, as FUR is increased, the hot spot location moves closer to the fuel gas inlet. One of the performance criteria requires that the peak cell temperature be lower than the sintering temperature used in the manufacturing process, which is approximately 1600 °K. Results obtained using the best possible V-I curve indicate that the array sizes could exceed 20 cm x 20 cm and still satisfy the hot spot requirement. For cases where the estimated V-I curve was applied, however, the peak temperature rose above 1600 °K for cell dimensions as small as 5 cm x 5 cm, as seen in the diagram.

Since the location of the minimum array temperature is invariant, both the magnitude and the relative location of the maximum temperature must be considered when assessing thermal stresses. At large FUR values, the peak temperature is in close proximity to the minimum temperature and large thermal gradients will be developed, the severity of which depends on the materials used.

Results from the computer model show that array dimensions for a cross-flow monolithic fuel cell can be restricted as a result of non-uniform temperature distributions. Improvements in the V-I curve will alleviate much of this problem. Also, a range of allowable reactant utilization ratios will be established when a set of operational parameters are specified.

References

[1] Feduska, W., et al.: High-Temperature, Solid Oxide Electrolyte Fuel Cell Power Generation System. DOE/ET-17089-T3, June 1982.

[2] Fee, D.C., et al.: Monolithic Fuel Cell Development. CONF-861008-6, 1986.
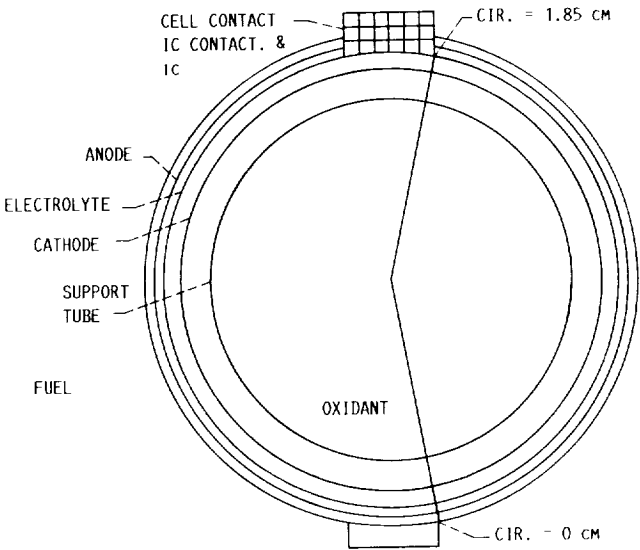
Acknowledgment

FIGURE 1. - MODEL USED TO ANALYZE CIRCUMFERENTIAL CURRENT DENSITY
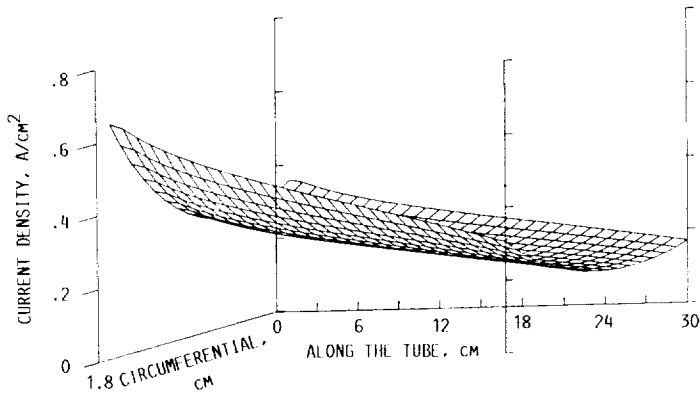DISTRIBUTIONS FOR TUBULAR SOFC.

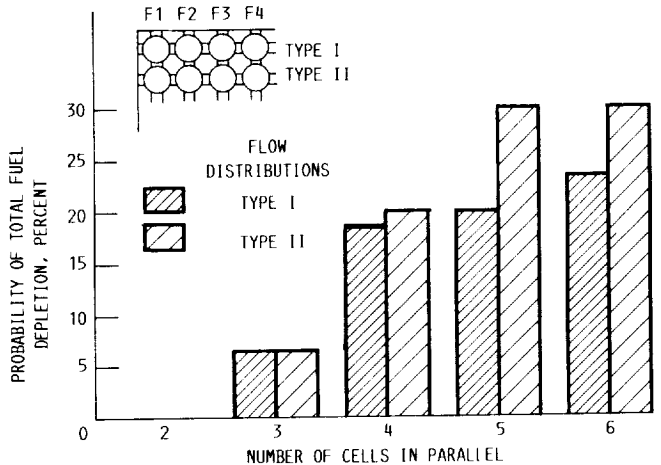FIGURE 2. - TUBULAR SOFC CURRENT DENSITY PROFILE (ISOTHERMAL).

FIGURE 3. - PROBABILITY OF FUEL DEPLETION (OF THE EDGE CELLS)
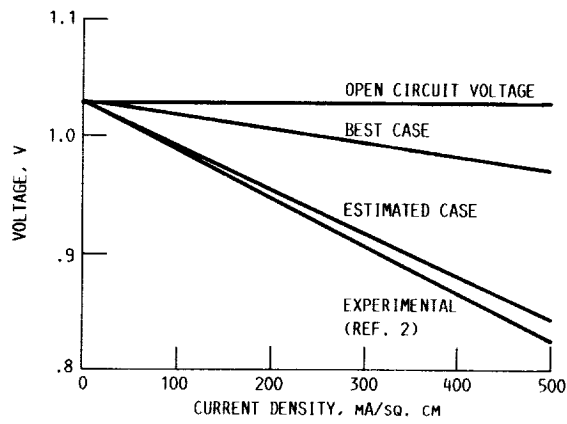VERSUS CELL CONFIGURATION.
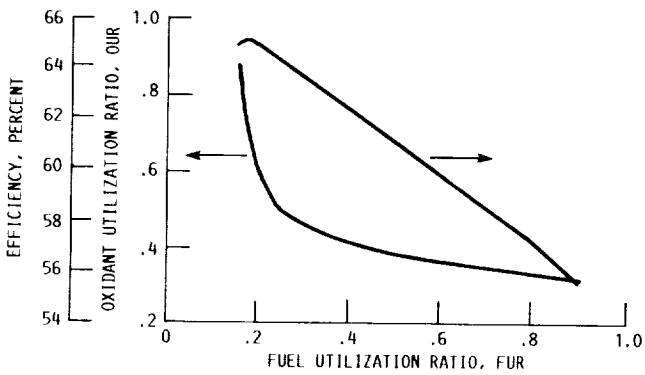
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FIGURE 4. - MONOLITHIC SOFC V-I CURVES.

OPEN CIRCUIT VOLTAGE
BEST CASE
ESTIMATED CASE
EXPERIMENTAL
(REF. 2)

FIGURE 5. - OUR AND EFFICIENCY VERSUS FUR.

CROSS FLOW CONFIGURATION
(5 CM X 5 CM)
OUR = 0.71, FUR = 0.20
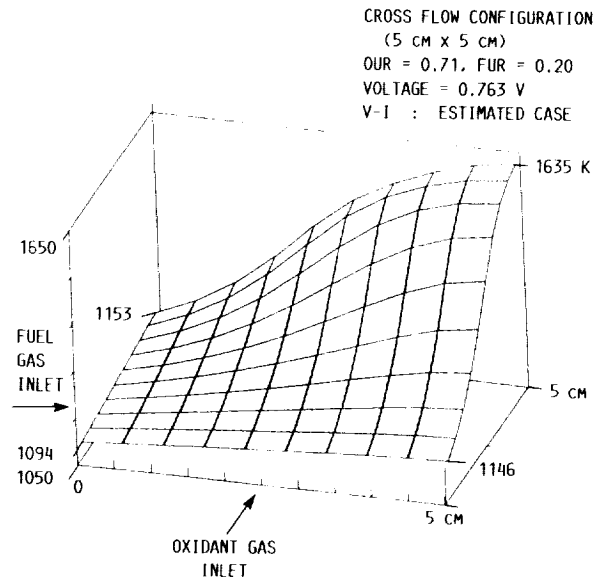VOLTAGE = 0.763 V
V-I : ESTIMATED CASE

FUEL
GAS
INLET

OXIDANT GAS
INLET

FIGURE 6. - MONOLITHIC SOFC TEMPERATURE DISTRIBUTION FOR
EXAMPLE CASE.

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Report Documentation Page

1. Report No. NASA CR-182188 DOE/NASA/0017-5	2. Government Accession No.	3. Recipient's Catalog No.
4. Title and Subtitle Mathematical Modeling of Solid Oxide Fuel Cells		5. Report Date August 1988
		6. Performing Organization Code
7. Author(s) Cheng-Yi Lu and Thomas M. Maloney		8. Performing Organization Report No. E-4319
		10. Work Unit No. 778-17-01
9. Performing Organization Name and Address Cleveland State University Department of Chemical Engineering Cleveland, Ohio 44115		11. Contract or Grant No. NCC 3-17
		13. Type of Report and Period Covered Contractor Report Final
12. Sponsoring Agency Name and Address U.S. Department of Energy Office of Coal Utilization and Extraction Washington, D.C. 20545		14. Sponsoring Agency Code

15. Supplementary Notes

Prepared under Interagency Agreement DE-AI21-80ET17088. Project Manager, Robert Wagner, Power Systems Integration Office, NASA Lewis Research Center, Cleveland, Ohio 44135. Prepared for the 1988 Fuel Cell Seminar, sponsored by the National Fuel Cell Coordinating Group, Long Beach, California, October 23-26, 1988.

16. Abstract

Development of predictive techniques, with regard to cell behavior, under various operating conditions is needed to improve cell performance, increase energy density, reduce manufacturing cost, and to broaden utilization of various fuels. Such technology would be especially beneficial for the solid oxide fuel cell (SOFC) at its early demonstration stage. This paper describes the development of computer models to calculate the temperature, CD, and reactant distributions in the tubular and monolithic SOFCs. Results indicate that problems of nonuniform heat generation and fuel gas depletion in the tubular cell module, and of size limitations in the monolithic (MOD 0) design may be encountered during FC operation.

17. Key Words (Suggested by Author(s)) Solid oxide fuel cells; Tubular; Monolithic; Performance; Computer model	18. Distribution Statement Unclassified – Unlimited Subject Category 44 DOE Category UC-97D		
19. Security Classif. (of this report) Unclassified	20. Security Classif. (of this page) Unclassified	21. No of pages 10	22. Price* A02