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ELECTROCHEMICAL CARBON DIOXIDE CONCENTRATOR: MATH MODEL

FINAL REPORT

by
R.D. Marshall, F.H. Schubert
and J.N. Carlson

August, 1973

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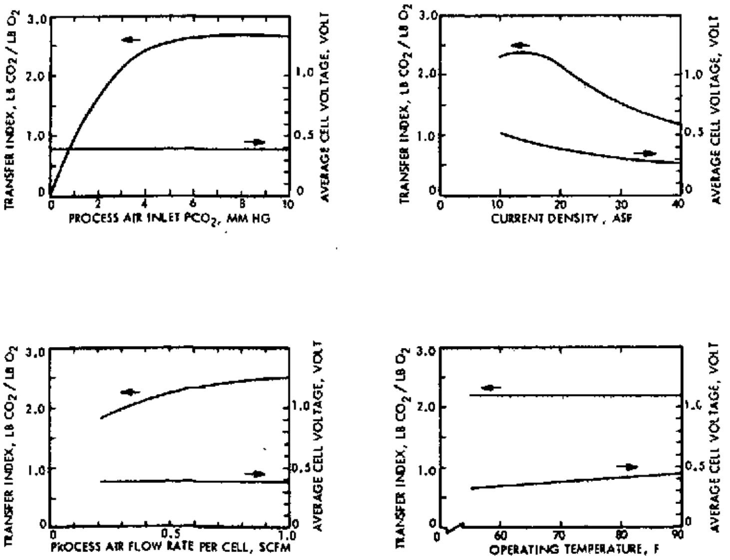
MATH MODEL SIMULATION CURVES



Prepared Under Contract No. NAS2-6478

by

Life Systems, Inc.
Cleveland, Ohio 44122

for

AMES RESEARCH CENTER

National Aeronautics & Space Administration

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I

FOREWORD

The development work described herein was conducted by Life Systems, Inc. during the period May, 1972 to August, 1973 as part of NASA Contract NAS2-6478. The Program Manager was Richard D. Marshall. Technical support was provided by:

John C. Bronikowski - Supporting Experiments

Jan Carlson - Computer Programming and Logic

Jon Schneider - Supporting Experiments

Franz H. Schubert - Administrative Support

The work performed on the Mathematical Model was funded by Johnson Space Center through Ames Research Center as an additional task to the development of a Six-Man, Self-Contained, Carbon Dioxide Concentrator Subsystem (Contract NAS2-6478).

Direct technical monitorship was provided by W. E. Ellis, Chief, Environmental and Thermal Systems Section, Crew Systems Division, Johnson Space Center, Houston, Texas. Technical support was provided at Johnson Space Center by Dr. C. H. Lin and Dr. J. Winnick.

The Contract Technical Monitor was P. D. Quattrone, Chief, Environmental Control Research Branch, NASA Ames Research Center, Moffett Field, California.

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SUMMARY

A steady-state computer simulation model of an Electrochemical Depolarized Carbon Dioxide Concentrator (EDC) has been developed. The mathematical model combines EDC heat and mass balance equations with empirical correlations derived from experimental data to describe EDC performance as a function of the operating parameters involved. The model is capable of accurately predicting performance over EDC operating ranges. Model simulation results agree with the experimental data obtained over the prediction range.

Eight experiments were conducted in support of the mathematical model to study the effect of the cell matrix on cell internal resistance (formation factor); anode gas pCO_2 levels; process air flow rate; current density, process air inlet pCO_2; matrix thickness; electrode thickness; thermal conditions within a cell; and the transient response of a cell to changes in process air inlet pCO_2, current density and air flow rate.

A computer program was written for the numerical solution of the mathematical expressions describing system performance. The program was written in Fortran IV for use on a Univac 1108 Digital Computer.

INTRODUCTION

In an Electrochemical Depolarized Carbon Dioxide Concentrator (EDC) numerous physical, chemical and electrochemical processes interact simultaneously. These processes can be experimentally defined and characterized mathematically for computerized solution to predict EDC performance as a function of the operating parameters involved. In addition to predicting performance, the mathematical model can be used to optimize subsystem designs and performance, and aid in integrating an Electrochemical Carbon Dioxide Concentrator Subsystem with other regenerative life support subsystems.

In parallel to the development of a Six-Man Electrochemical Carbon Dioxide Concentrator Subsystem(1), a program was completed to

1. define the electrochemical carbon dioxide (CO_2) concentration process to analytically determine the relationship between EDC performance and the operating parameters and to provide a basis for assumptions made;
2. perform eight experiments to supplement previously obtained data and to support the development of an analytical mathematical model;(2)
3. transcribe the experimentally defined functional relationships between operating parameters and EDC performance into mathematical expressions (empirical correlations) for computerized solution; and

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(1) All references cited are listed at the end of the report.

4. prepare a computer program to predict EDC performance by solving the empirical correlations obtained and EDC heat and mass balance equations as a function of the operating parameters involved.

The theoretical work completed was used to gain an understanding of the processes involved in the electrochemical concentration of CO_2 and to define where experimental results were needed. The computer program prepared was based on experimental performance results and did not necessarily incorporate the theoretical work completed.

The following sections summarize the results of the program.

ELECTROCHEMICAL CARBON DIOXIDE CONCENTRATION

Carbon dioxide is removed from a flowing air stream as it passes over the cathode of an EDC cell. Each cell consists of two porous electrodes separated by a porous matrix containing an aqueous solution of cesium carbonate (Cs_2CO_3). Plates adjacent to the electrodes provide passageways for distribution of the process gases and electrical current over the electrode surfaces. The specific electrochemical and chemical reactions are detailed in Figure 1.

Moist air containing CO_2 is fed into the cathode where the electrochemical reaction of oxygen (O_2) in the air, water (H_2O) and electrons forms hydroxyl ions (OH^-). Hydroxyl ions then react with the CO_2 forming carbonate ions ($CO_3^=$). The output from the cathode compartment is moist air at a reduced CO_2 partial pressure (pCO_2). At the anode side hydrogen (H_2) is fed into the cell. The electrochemical reaction of the H_2 and OH to form H_2O and electrons decreases the concentration of OH in the electrolyte at the anode. Carbon dioxide is produced in the resulting equilibrium shift completing its transfer from the cathode compartment to the anode compartment. The output from the anode compartment is CO_2 mixed with unreacted H_2. The overall reaction is exothermic and is accompanied by the formation of electrical energy.

EDC Performance

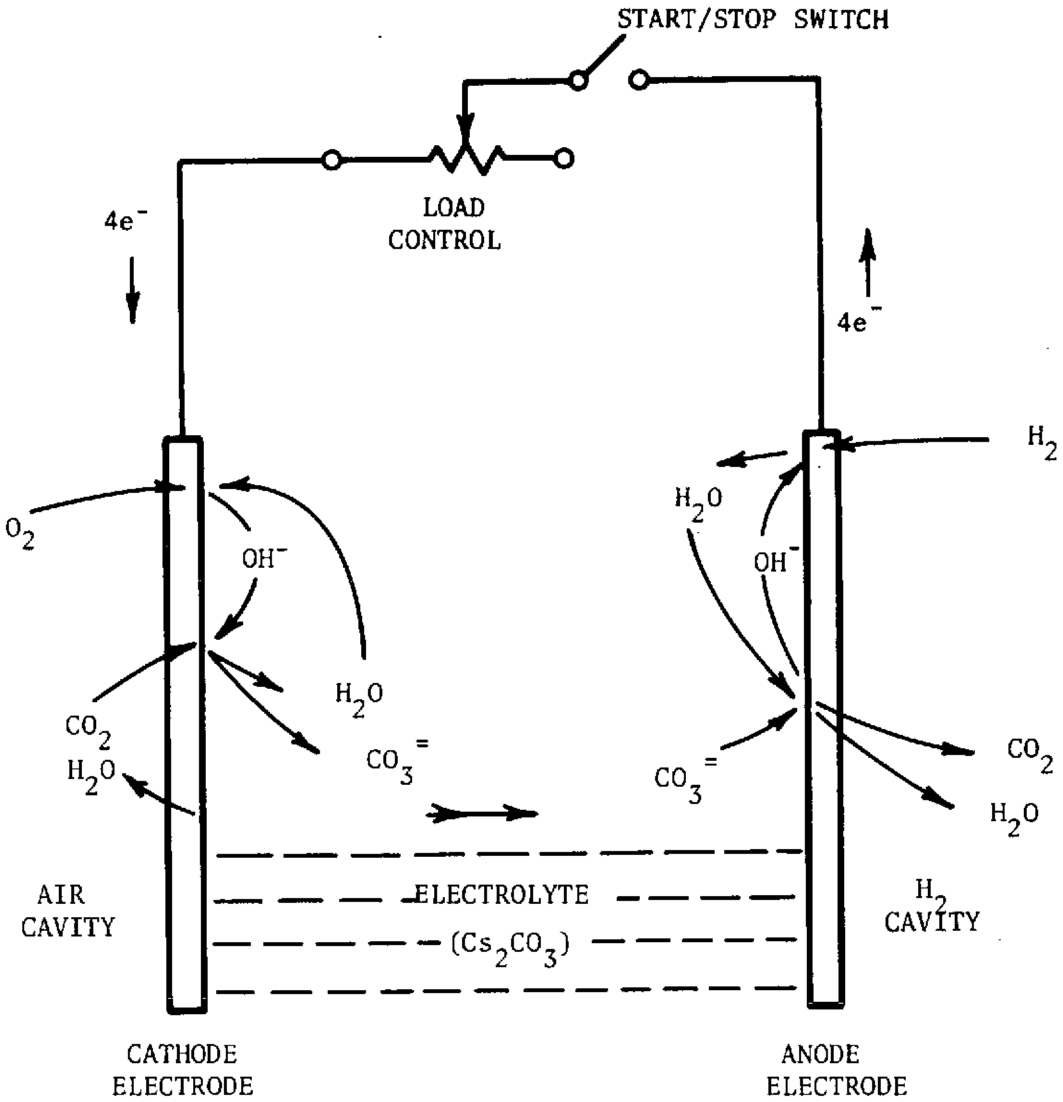
The performance of an EDC is reflected by CO_2 removal efficiency and electrical efficiency.

Carbon Dioxide Removal Efficiency

Inspection of the overall reaction as based on the $CO_3^=$ transfer mechanism

$$O_2 + 2CO_2 + 2H_2 \longrightarrow 2CO_2 + 2H_2O + \text{Electrical Energy} + \text{Heat}$$

shows that two moles of CO_2 can be transferred for one mole of O_2 consumed. This represents a CO_2 removal efficiency of 100%. The equivalent weight ratio is 2.75 lb of CO_2 removed for each pound of O_2 consumed. This ratio has been referred to as the Transfer Index (TI).



CATHODE REACTIONS:

$O_2 + 2H_2O + 4e^- = 4OH^-$

$4OH^- + 2CO_2 = 2H_2O + 2CO_3^=$

ANODE REACTIONS:

$2H_2 + 4OH^- = 4H_2O + 4e^-$

$2CO_3^= + 2H_2O = 4OH^- + 2CO_2$

OVERALL REACTION:

$O_2 + 2CO_2 + 2H_2 \longrightarrow 2CO_2 + 2H_2O$ + Electrical Energy + Heat

FIGURE 1 ELECTROCHEMICAL AND CHEMICAL REACTIONS

To gain a better understanding of the dependency of the CO_2 removal process and, hence, removal efficiency upon the operating parameters involved, the CO_2 mass transfer process was subdivided into five steps. They are (1) air cavity transfer, (2) cathode reactions, (3) electrolyte transfer, (4) anode reactions, and (5) H_2 cavity transfer.

Air Cavity Transfer. Carbon dioxide in the process air stream diffuses in the cathode compartment to the electrode surface and then through the electrode pores to the gas-electrolyte interface. The air cavity CO_2 transfer rate can be estimated using a convective mass transfer coefficient. The equation for air cavity CO_2 transfer is

$$N_{CO_2} = (k_c)(A)(M_{CO_2})(pCO_2 - pCO_2^{o})/RT$$

Where

N_{CO_2} = CO_2 transferred, lb/hr

k_c = convective mass transfer coefficient, ft/hr

A = transfer area, in^2

pCO_2 = CO_2 partial pressure in air stream, psia

pCO_2^{o} = CO_2 partial pressure at the gas-electrolyte interface, psia

M_{CO_2} = molecular weight of CO_2, lb/lb mol

R = Universal Gas Constant, ft-lb/lb mol-R

T = absolute temperature, R

Air cavity CO_2 mass transfer rate, therefore, depends on pCO_2; k_c, a function of process air flow rate; cathode compartment and electrode geometry and the physical properties and diffusion coefficients of the gases involved; temperature; and pressure. The physical properties and diffusion coefficients can be assumed constant with negligible error over typical EDC operating ranges in temperatures (60-80F) and pressure (14.7 psia). For a given EDC cell geometry and normal temperature and pressure conditions, air cavity CO_2 mass transfer rate is assumed to be only a function of process air flow rate and pCO_2.

Cathode Reactions. Carbon dioxide reacts with electrochemically-generated OH^- at the cathode to form $CO_3^=$ in two consecutive reactions(3)

$$CO_2 + OH^- \rightleftharpoons HCO_3^-$$

$$HCO_3^- + OH^- \rightleftharpoons CO_3^= + H_2O$$

In strong basic solutions the equation for the reaction rate is(4)

$$\frac{-d\,[CO_2]}{dt} = k\,[CO_2][OH^-]$$

Where

k = second order rate constant, 1/mol-sec

$[CO_2]$ = CO_2 concentration, mol/l

$[OH^-]$ = OH^- concentration, mol/l

The CO_2 available for reaction is in equilibrium with pCO_2^o at the gas-electrolyte interface in the electrode pores. The OH^- available for reaction is a function of cell current density, and k is a function of temperature. For the cathode reactions, CO_2 transfer rate is a function of pCO_2, cell current density and temperature.

Electrolyte Transfer. Carbon dioxide as $CO_3^=$ and unreacted OH^- diffuse through the bulk electrolyte to the anode. Since current is carried by $CO_3^=$, CO_2 mass transfer is the sum of molecular and convective diffusion and ionic migration under the electrical potential gradient between the two cell electrodes. The equation describing the transfer of charged species through electrolyte solutions is given by the Nernst-Planck equation(2)

$$N_j = - D_j \frac{dC_j}{dx} - z_j F u_j C_j \frac{d\phi}{dx} + C_j v$$

Where

D_j = diffusion coefficient of j

z_j = electrical charge of j

F = Faraday's constant

u_j = electrical mobility

C_j = concentration of j

ϕ = electrical potential

x = transfer distance

v = bulk fluid velocity

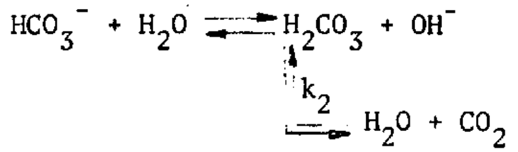
For transfer through the electrolyte, v can be assumed to be zero. The mass transfer rate through the electrolyte then is a function of the diffusion coefficients, electrolyte composition, matrix structure, temperature and current density.

Anode Reactions. Carbonate ions react with electrochemically formed H_2O to form CO_2. As H_2O is formed the equilibrium shifts from $CO_3^=$ to bicarbonate ions (HCO_3^-).

$$H_2O + CO_3^= \rightleftharpoons HCO_3^- + OH^-$$

At the lower anolyte pH levels, two parallel reaction mechanisms can take place

$$1.\quad HCO_3^- \underset{}{\overset{k_1}{\rightleftharpoons}} CO_2 + OH^-$$



$$2.\quad HCO_3^- + H_2O \rightleftharpoons H_2CO_3 + OH^- \qquad H_2CO_3 \overset{k_2}{\rightleftharpoons} H_2O + CO_2$$

The equation describing the reaction rate is

$$\frac{d[CO_2]}{dt} = \frac{k_1}{K_1}\,[HCO_3^-] - k_1\,[CO_2][OH^-] + k_2\,[H_2CO_3] - \frac{k_2}{K_2}\,[CO_2](a_{H_2O})$$

Where

k_1, k_2 = reaction rate constants

K_1, K_2 = equilibrium constants

a_{H_2O} = activity of H_2O

The concentration of dissolved CO_2 is in equilibrium with the anode gas pCO_2 at the gas-electrolyte interface in the electrode pores. For the anode reactions, CO_2 transfer rate is a function of anode gas pCO_2, cell current density and temperature.

Hydrogen Cavity Transfer. Carbon dioxide diffuses through the electrode pores and into the anode gas stream. Hydrogen cavity CO_2 mass transfer rate can be estimated using a convective mass transfer coefficient similar to the air cavity mass transfer coefficient. The equation for H_2 cavity CO_2 transfer is

$$N_{CO_2} = (k_c)(A)(M_{CO_2})(pCO_2^{\,o} - pCO_2)/RT$$

Where

pCO_2, $pCO_2^{\,o}$ and k_c are evaluated for the H_2 cavity conditions.

Electrical Efficiency

The electrical energy produced by the electrochemical reaction in the EDC is a function of the current density and the cell voltage. The theoretical open-circuit voltage is 1.23 volts. In practical applications, and with current flowing, cell voltages of less than 1.23 volts result. Electrical efficiency is therefore reflected by cell voltage with high cell voltage representing high electrical efficiency.

Cell voltage is the sum of the reversible electrochemical reaction voltages (E_R) overvoltages (E_O) and concentration polarizations (E_C) at each electrode and the voltage loss due to the internal resistance of the electrolyte-filled matrix (E_{IR}). The expressions for E_R, E_O and E_C can be derived from thermodynamic considerations. However, E_{IR} depends on electrolyte matrix conductivity for a given matrix material and configuration (i.e., matrix compression, porosity, etc.).

A general equation can be used to describe cell voltage as a function of cell current density and temperature(5)

$$E = E_R - (a \ln i + bi + c \ln (\frac{i_L - i}{i_L}) + d)$$

Where

a, b, c and d = constants

E = cell voltage, volt

i = cell current density, ASF

T = cell temperature, F

i_L = limiting current density, ASF

The constants in the equation depend on temperature and the electrode-electrolyte matrix-electrode structure and properties and can be found using cell performance data for a specific EDC design. The limiting current density depends on anode gas flow rate and pH_2, and air flow rate and pO_2.

Operating Parameters Affecting EDC Performance

Six major operating parameters affect EDC performance. They are

1. pCO_2 in the air supplied to the cell,
2. current density at which the cell operates,
3. air flow rate through the cathode compartment,
4. pCO_2 in the H_2 stream,
5. H_2 flow rate through the anode compartment, and
6. temperature level at which the cell operates.

The effect of each parameter on CO_2 removal and electrical efficiencies has been characterized experimentally.

EDC Hardware

The mathematical model developed is based on Life Systems' EDC cell design.

Figure 2 is a schematic of the concentrator cell. The cell consists of a cathode and an anode gas compartment, two current collectors with gas compartment spacers, two electrodes, and an electrolyte matrix. Figure 3 is a photograph of the cell parts. The basic materials of construction are Life Systems' baseline electrodes, asbestos electrolyte matrix, nickel expanded metal (Exmet) gas compartment spacers, nickel current collectors, and polysulfone structural cell frames. The cell utilizes externally air-cooled fins attached to the anode current collector to remove the waste heat generated by the electrochemical reactions. The materials of construction and cell dimensions are summarized in Table 1.

EDC Control

Steady-state EDC operation requires that H_2O and heat generated in the electrochemical cell reactions be removed to maintain cell moisture balance. Cell temperature is controlled at a set differential temperature above the process air inlet dew point temperature. This control scheme allows the process air humidity and cell electrolyte concentration to remain in balance as generated H_2O and heat are removed.

Water Removal

The H_2O generated in the electrochemical reactions must be removed from the cell by the process air stream. (Some H_2O is removed in the H_2 stream but due to the low flow rates this can be assumed negligible.) For steady-state it is necessary to balance the amount of H_2O that is added to the process air stream such that the electrolyte concentration remains constant. The equation for the H_2O produced in an EDC is

$$W = 7.4 \times 10^{-4} (N)(I)$$

Where

W = H_2O produced, lb/hr

N = number of series-connected cells

I = cell current, amp

Process air humidity conditions in which all the H_2O is not removed would result in a decrease in the electrolyte concentration. The resulting volume increase may cause electrolyte to be deposited in the gas cavities. Should more than the electrochemically-formed H_2O be removed, the electrolyte concentration would increase and the resulting volume decrease may cause electrolyte precipitation or electrolyte to be pulled out of the electrode pores (the result is a cell failure allowing gas to cross from one cavity to another).

Heat Removal

For the electrochemical reactions involved, the cell voltage derived from the heat of reaction, is 1.25 volt. The net heat produced by an EDC is given by the following equation.

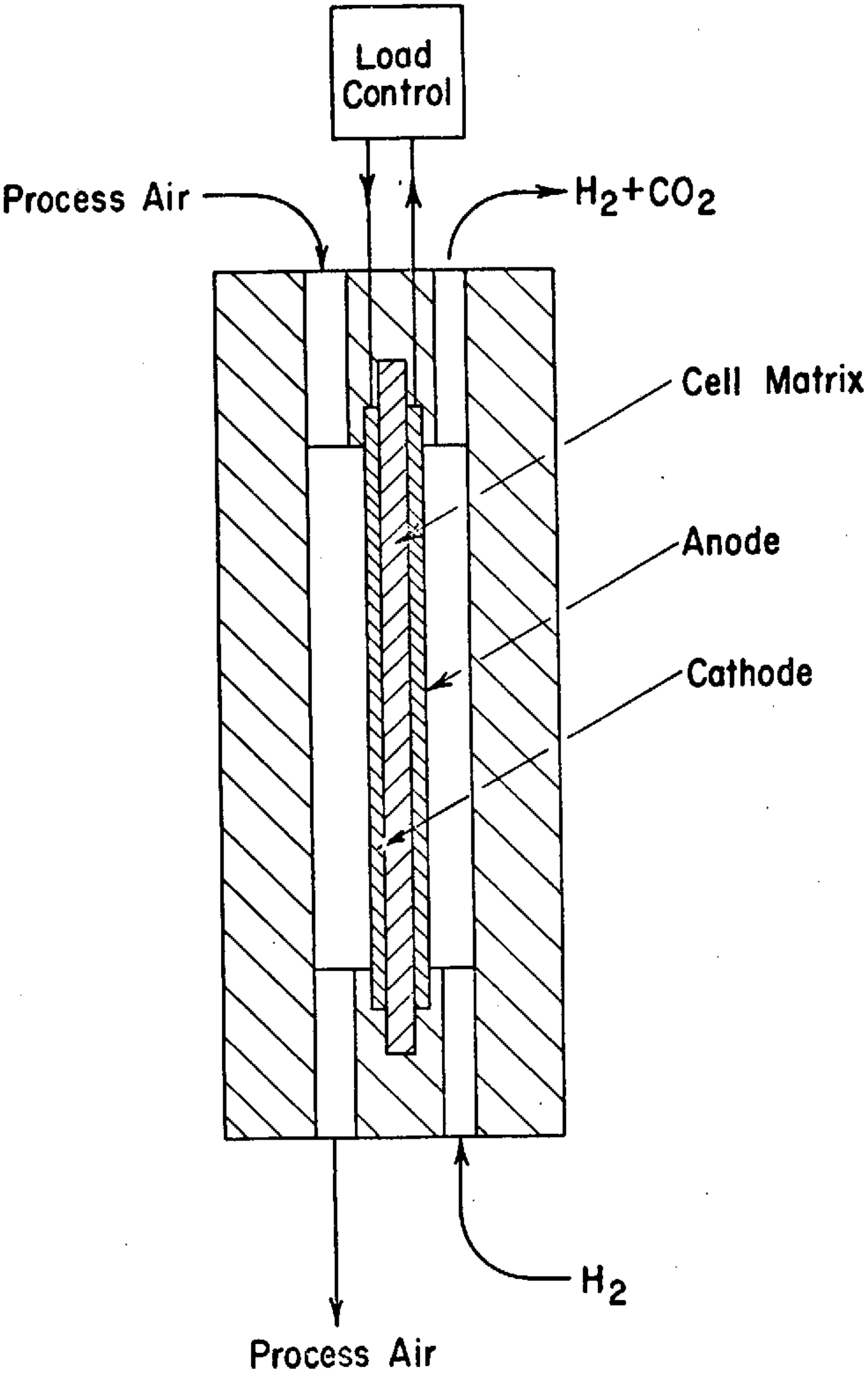


FIGURE 2 EDC CELL SCHEMATIC

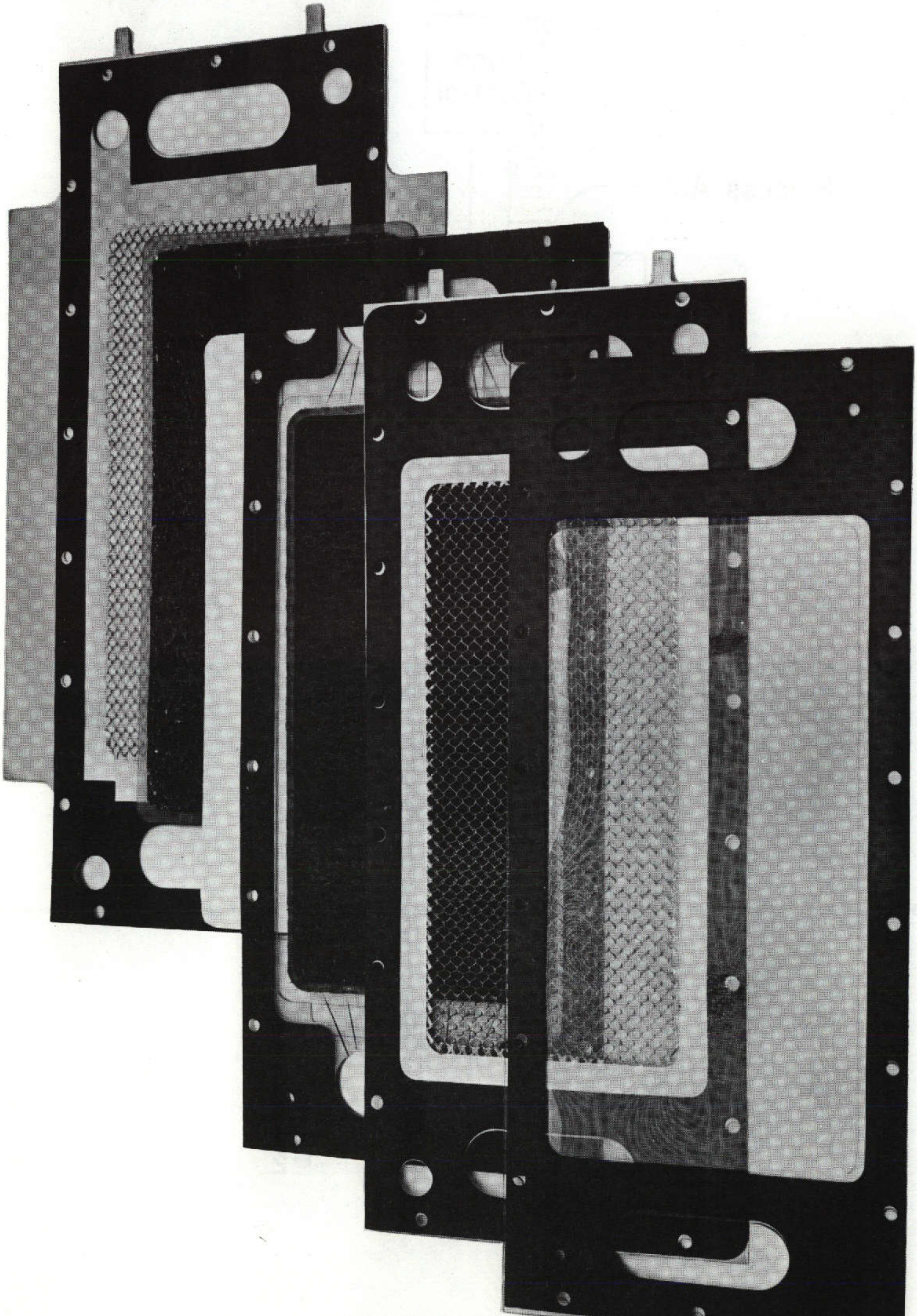


FIGURE 3 EDC CELL PARTS

TABLE 1 EDC CELL CHARACTERISTICS

Active Area (per cell)	0.244 Ft^2 (4.1 x 8.6 In)
Air Cavity Height	0.082 In
H_2 Cavity Height	0.062 In
Cell Matrix	0.030 In, Asbestos
Cell Frames	Injection-Molded Polysulfone
H_2 Current Collector	Nickel 200
O_2 Current Collector	Nickel 200
Gaskets	Ethylene Propylene

$$Q = (1.25-E)\ NI \times 3.419$$

Where

Q = heat produced, Btu/hr

I = the current, amp

E = cell voltage, volt

The net heat produced is absorbed by the process air, the H_2 stream and the cooling air so that

$$Q = \Delta H_a + \Delta H_h + \Delta H_c$$

Where

ΔH_a = heat removed by the process air

ΔH_h = heat removed by the process H_2

ΔH_c = heat removed by the process cooling air

TEST PROGRAM

A successful Test Program supplemented previously obtained performance data for 1-, 3-, 15- and 90-cell EDC designs and produced specific operating data for current density, pCO_2 and air flow variations that would aid in mathematically characterizing EDC performance.

The testing was parametric in nature and a single-cell EDC was used. The three-cell test facility also developed under NASA Contract NAS2-6478 was modified for single-cell testing and was used for the experiments. A schematic of the test facility is presented in Figure 4. Specifically, the test facility has the capability of varying process air flow rate, dew point and pCO_2, H_2 flow rate, current density and cell temperature.

A series of eight experiments were completed to support the EDC mathematical model development. They were

1. formation factor determination,
2. effect of anode gas pCO_2 variations,
3. air cavity mass transfer coefficient determination,
4. effect of low current density,
5. effect of matrix thickness,
6. effect of electrode thickness,

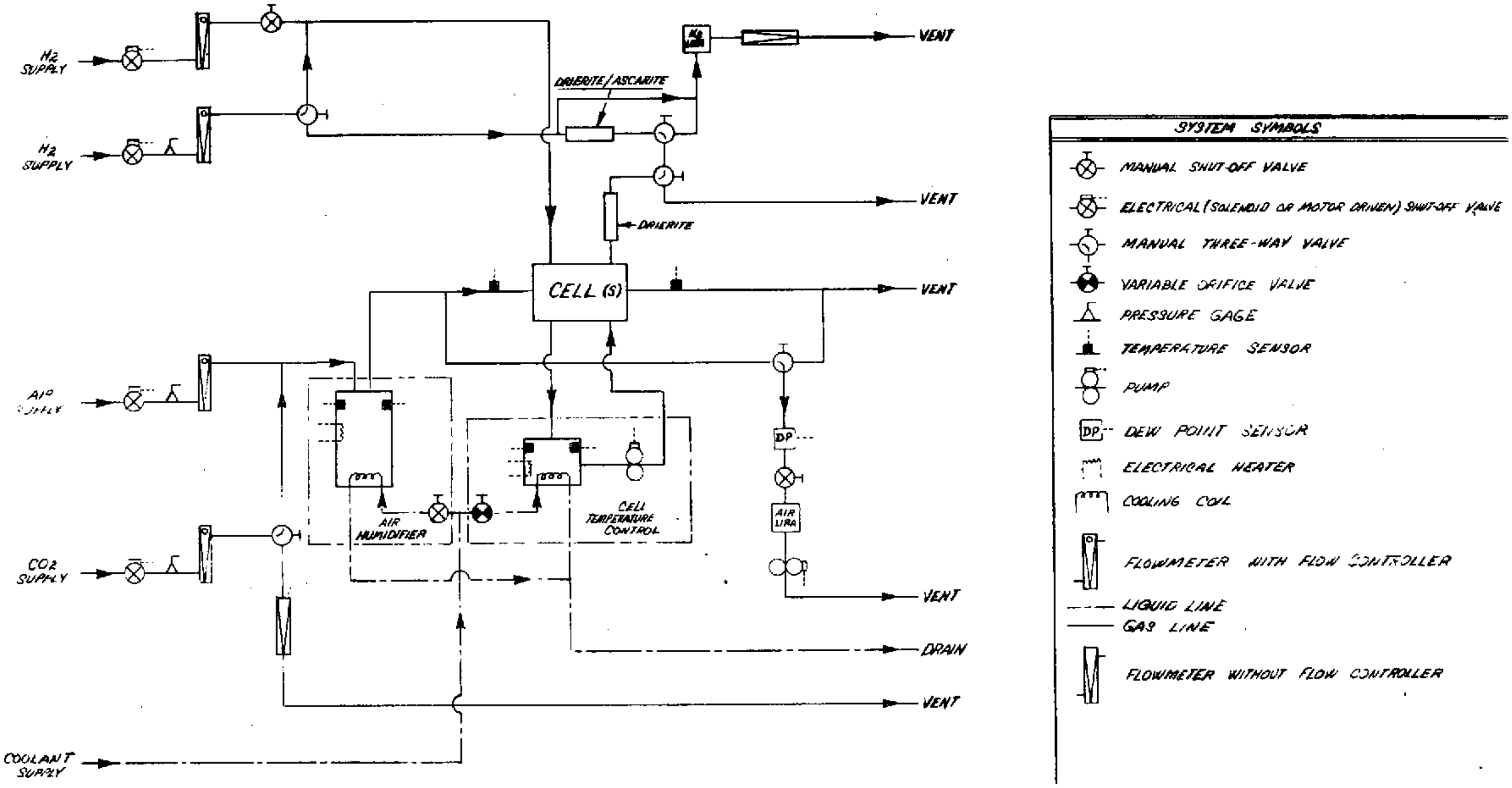


FIGURE 4 MATH MODEL TEST SETUP SCHEMATIC

7. EDC temperature profile determination (thermal gradient), and

8. EDC transient response to step changes in operating conditions.

The baseline test conditions of the experiment are given in Table 2. Table 3 summarizes the ranges over which the test parameters were varied.

Formation Factor Determination

The formation factor is defined as the ratio of the observed internal resistance (IR) of the cell (electrolyte-filled matrix) divided by the IR of the electrolyte. The formation factor for Life Systems' EDC cell design was determined for two concentrations of Cs_2CO_3. A Kordesch-Marko (K-M) Bridge was electrically connected in series with a single-cell EDC. The interrupted current from the K-M Bridge allowed the measurement of cell IR as a function of current density. The formation factor was calculated using the K-M Bridge IR measurements and Cs_2CO_3 conductivity data.

The results of the current density span for each Cs_2CO_3 concentration are presented in Figure 5. The formation factor for the 61.5% Cs_2CO_3 charge concentration was 6.2. For the 55% Cs_2CO_3 charge concentration the formation factor was found to be 5.8. (The formation factor calculations are given in Appendix A.) The results of the two formation factor determinations agree with experimental error and the average value, 6.0, can be used for the formation factor.

Effect of Anode Gas pCO_2 Variations

The effect of anode gas pCO_2 levels on EDC CO_2 removal and electrical efficiency was determined for a pCO_2 range of 0-690 mm Hg (at a total anode gas pressure of 760 mm Hg). Carbon dioxide was added to the inlet H_2 stream to simulate the various pCO_2 levels. The results of the experiment are presented in Figure 6. Carbon dioxide removal efficiency remained constant (TI = 1.98) through 640 mm Hg while cell voltage decreased steadily at approximately 0.2 millivolts per mm Hg. At 690 mm Hg or 90.8% by volume of CO_2 in the anode compartment, both TI and cell voltage decreased to 0 and 0.09 volts, respectively.

The minimum H_2 flow rate for normal EDC operation is 1.3 times the stoichiometric amount required by current. The maximum EDC anode gas pCO_2 level then is 585 mm Hg (assuming 1.3 x stoichiometric H_2 flow and TI = 2.75). For normal operating conditions the anode gas pCO_2 level is never greater than 253 mm Hg (assuming 3 x stoichiometric H_2 flow and TI = 2.75). Anode gas pCO_2 level then has a negligible effect on EDC performance causing only a slight decrease in cell voltage over the EDC's typical operating range.

Air Cavity Mass Transfer Coefficient Determination

The air cavity convective mass transfer coefficient was determined for an EDC. The convective mass transfer coefficient, k_c, was estimated using the following equation (see Appendix B for derivation)

$$k_c = AV^b$$

TABLE 2 BASELINE CONDITIONS FOR MATH MODEL EXPERIMENTS

Process Air Inlet	
Flow Rate	0.44-0.50 Scfm
Pressure	Ambient
Dew Point	50 ±2F
pCO_2	3.0 ±0.2 mm Hg
pO_2	3.1 Psia
Process H_2 Inlet	
Flow Rate	300 ±30 cc/Min
Pressure	Ambient
Cell	
Current (Current Density)	4.88 Amp (20 Asf)
Temperature	(Process air inlet dew point + 20) ±1F
Electrolyte	Cs_2CO_3
Charge Concentration	61.5 ±0.5% w/w

TABLE 3 SUMMARY OF MATH MODEL PARAMETRIC CHARACTERIZATION CURVES

Experiment No.	Description	Performance Variable(s)	Range[(a)]	Curve(s) Reflecting Results
1	Matrix Formation Factor	Current Density; Charge Concen.	10-40 Asf for 55% and 61.5%	Figure 5
2	Anode Gas pCO_2 Variations	Inlet anode gas pCO_2		Figure 6
3	Air Cavity Transfer Coefficient	Air Flow; pCO_2	0.2-0.8 Scfm for 1.0, 1.5, 2.0 and 10.2 mm Hg	Figure 7
4	Low Current Density Test	Current Density, pCO_2	5-30 Asf for 0.5, 3.0 and 9.0 mm Hg (nominal)	Figures 8 and 9
5	Thin Matrix Test	Current Density	10-40 Asf	Figure 10
6	Electrode Thickness	Current Density	10-40 Asf	Figure 11
7	Thermal Gradient	Current Density, Inlet Relative Humidity	80% and 63% RH at 20 Asf, 80% RH at 40 Asf	Figures 13 through 15
8	Transient Response	Operating Time after step changes in Current, Density, Air Flow and pCO_2	0-24 Hr for 20-30 Asf. 30-20 Asf, 0.48-0.91 Scfm. 0.91-0.49 Scfm, 3.0-5.5 mm Hg, 5.0-2.8 mm Hg	Figures 16 through 21

(a) Variable ranges not specified are at baseline conditions.

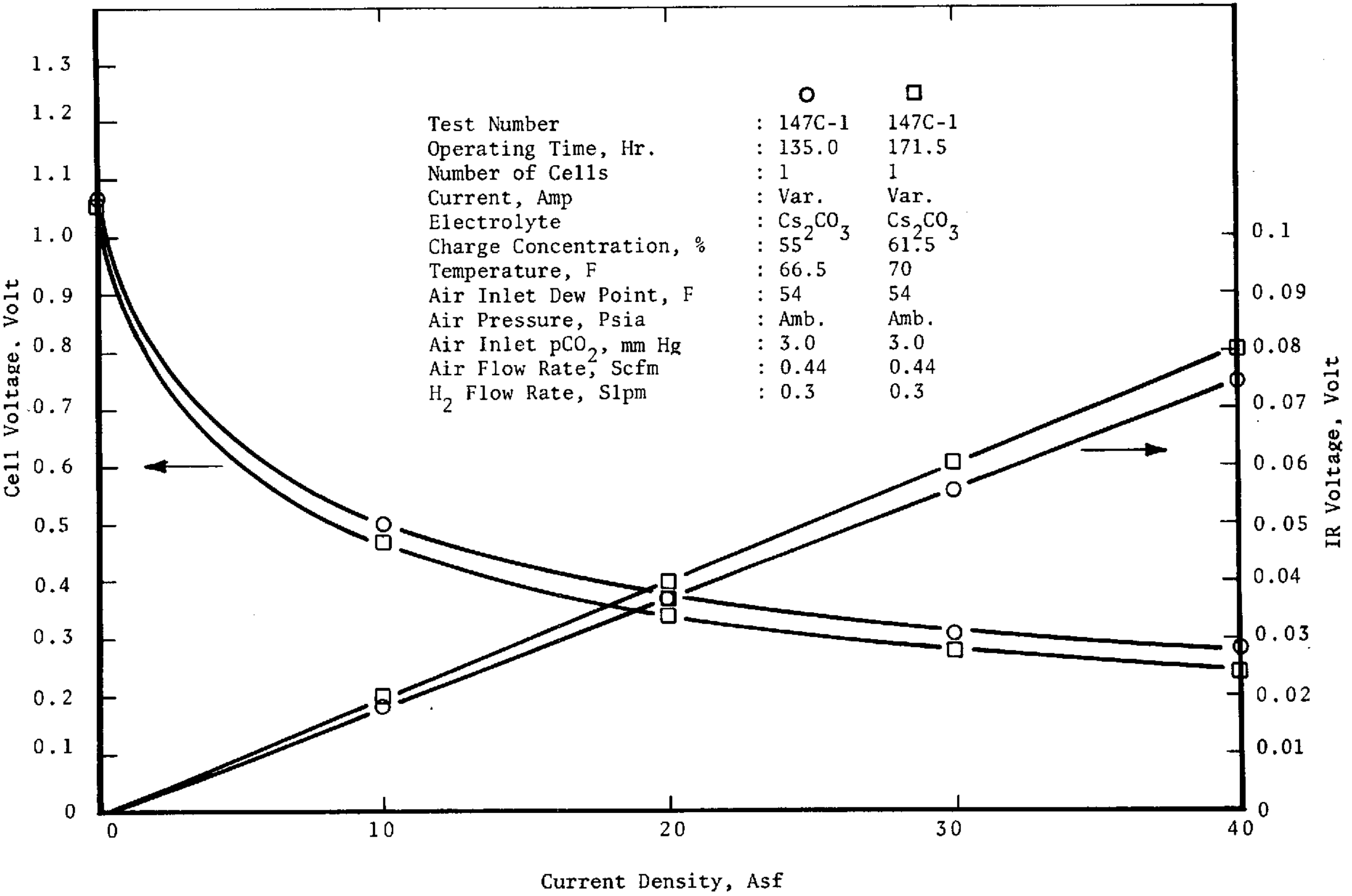


FIGURE 5 CELL VOLTAGE AND IR DROP AS A FUNCTION OF CURRENT DENSITY

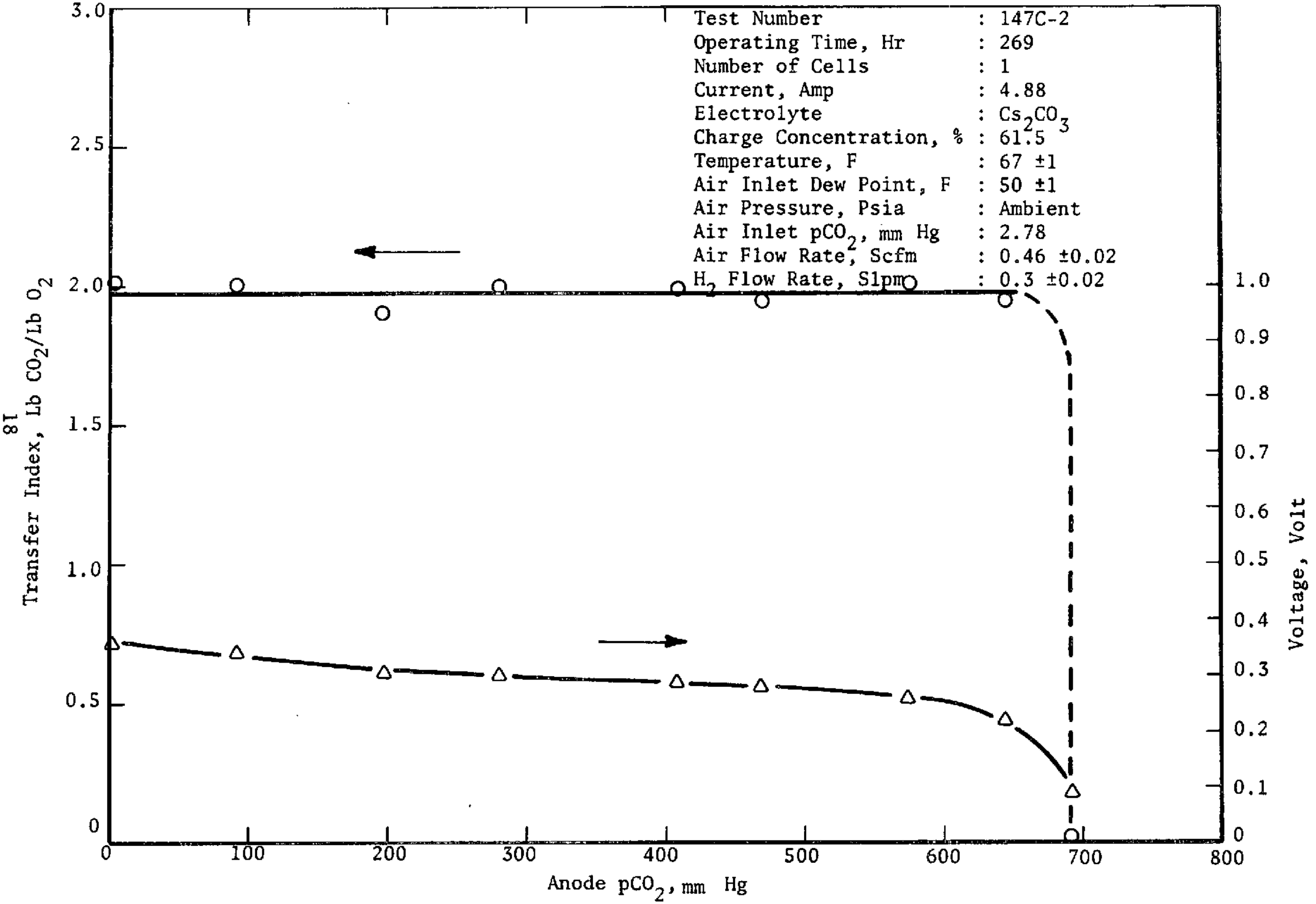


FIGURE 6 EFFECT OF ANODE GAS INLET PCO_2

Where

A, b = constants

V = volumetric air flow rate

At low inlet pCO_2 levels ($\leq$1.5 mm Hg at 20 ASF) air cavity mass transfer is rate-controlling and CO_2 removal is a function of the process air flow rate and pCO_2. At high pCO_2 levels ($\geq$5.0 mm Hg at 20 ASF) air cavity mass transfer is not rate-controlling and, hence, air flow rate has less effect on CO_2 removal. By measuring TI as a function of air flow rate at pCO_2 levels of 1.0, 1.5 and 2.0 mm Hg, A and b were calculated giving k_c as a function of process air flow rate. Also, the air flow test was run for 10.2 mm Hg to show that air flow had little effect on TI at higher pCO_2 levels. The results of the experiment are shown in Figure 7. The calculated values of A and b for 1.0, 1.5 and 2.0 mm Hg are

A = 113.9, b = 0.49 at 1.0 mm Hg

A = 90.8, b = 0.36 at 1.5 mm Hg

A = 88.3, b = 0.41 at 2.0 mm Hg

The correlation of data to the general equation derived for k_c was good, verifying that air cavity mass transport is rate-controlling at $\leq$1.5 mm Hg.

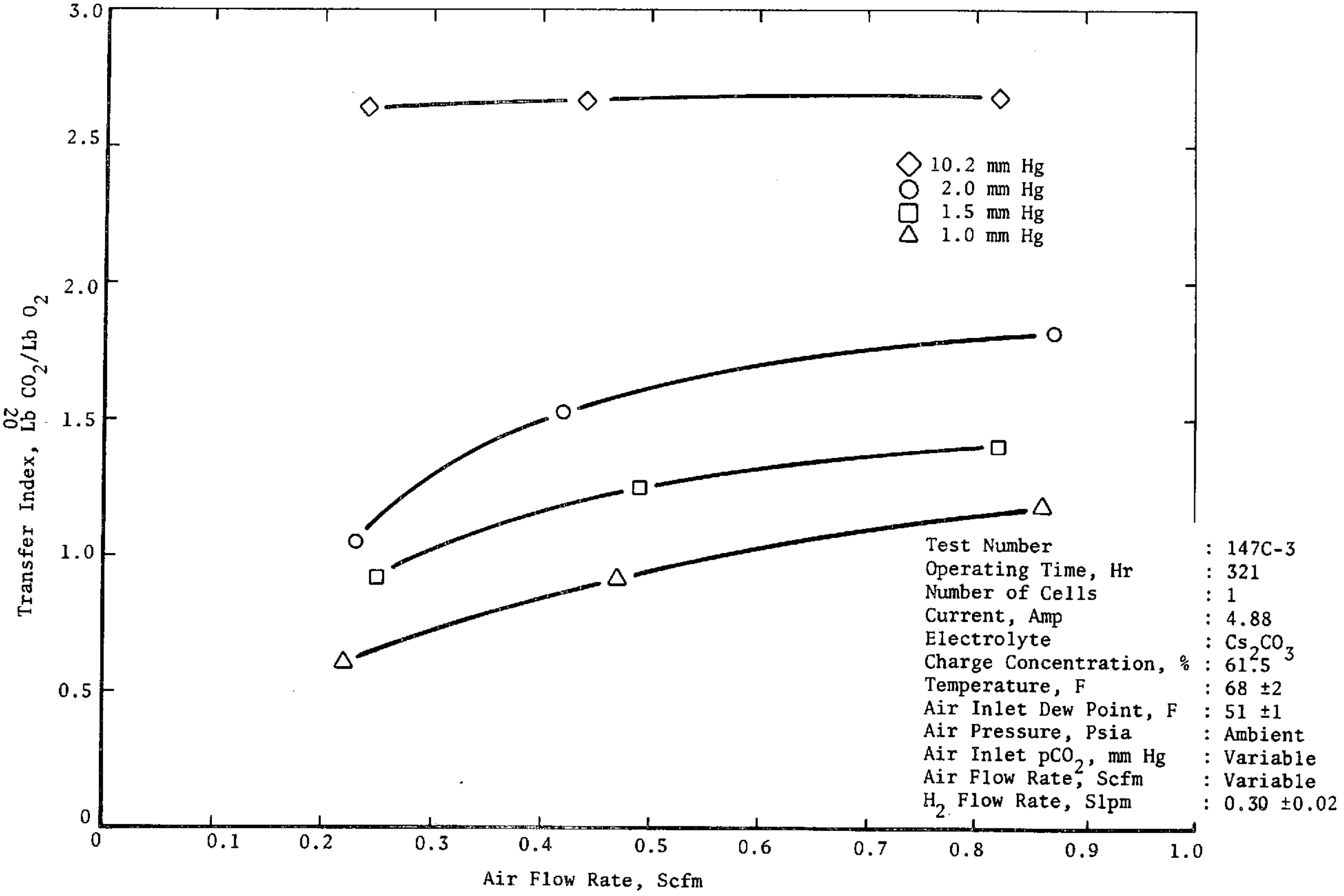
Effect of Low Current Density

At low current densities ($\leq$10 ASF) only a small amount of CO_2 is transferred making normal experimental transfer measurements inaccurate. For this experiment, a different technique was used to measure CO_2 transfer. A tube of ascarite was placed in the anode gas exit stream such that the H_2 and CO_2 flow entering the ascarite tube and the H_2 flow leaving the ascarite tube could be measured. Since all the CO_2 in the anode gas stream was absorbed by the ascarite, the difference in the flow rates of the two streams equalled the amount of CO_2 transferred.

EDC performance was determined as a function of current density for 5.0, 7.5, 10.0, 20.0 and 30.0 ASF at 0.5, 3.0 and 9.0 mm Hg (nominal) inlet pCO_2 levels. The results of the experiment are presented in Figure 8. These results were cross-plotted in Figure 9 to show the effect of current density on EDC performance at a given pCO_2 level. The results of the experiment for 20 and 30 ASF agreed with results previously obtained for TI as a function of current density and pCO_2.

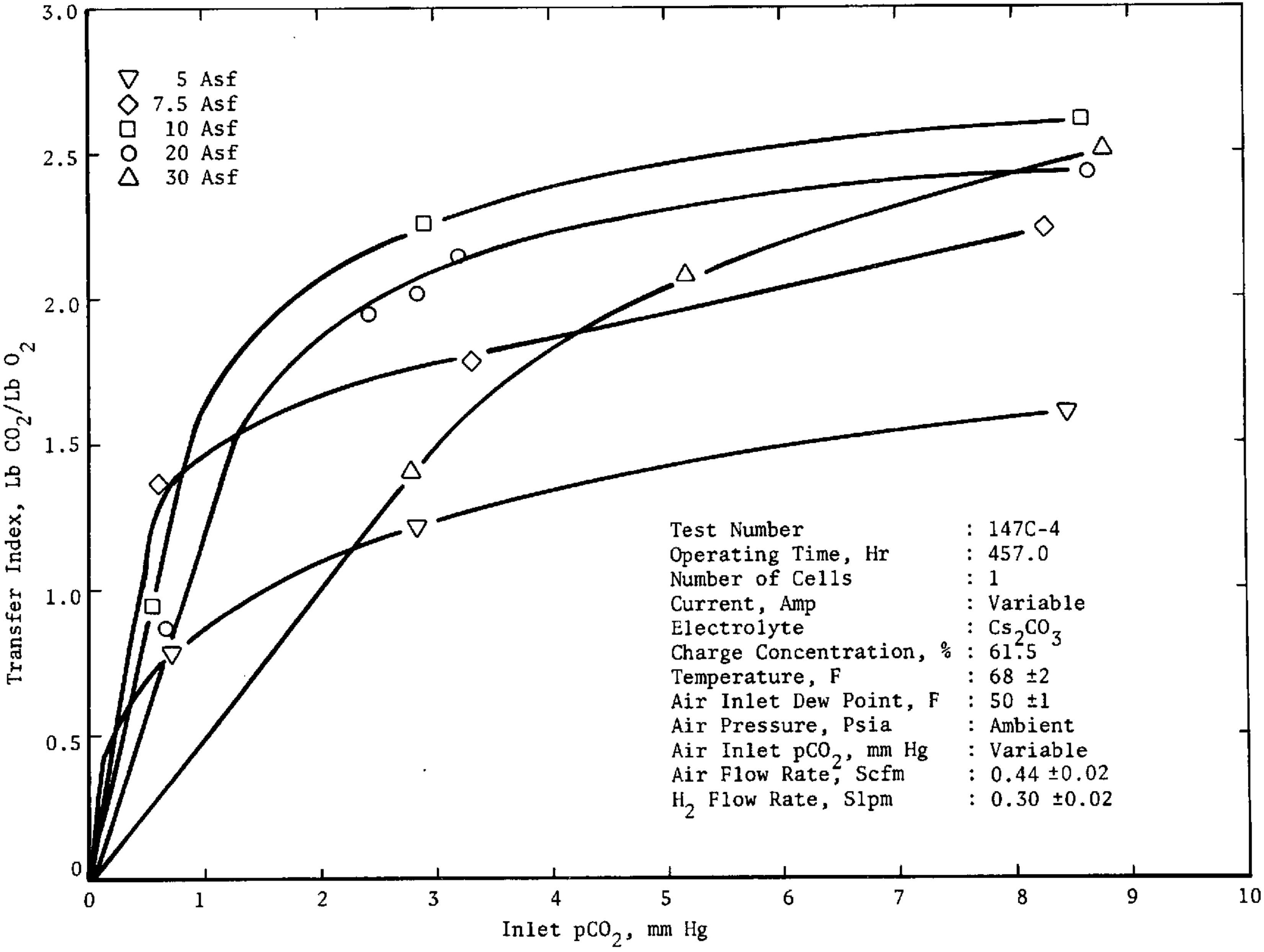
Effect of Matrix Thickness

EDC performance was determined as a function of current density for a 0.010-inch thick asbestos matrix as opposed to the standard 0.030-inch matrix used in Life Systems' EDC cell design. The results of the experiment are presented in Figure 10. The CO_2 removal efficiency was lower for the thinner matrix



Test Number : 147C-3
Operating Time, Hr : 321
Number of Cells : 1
Current, Amp : 4.88
Electrolyte : Cs_2CO_3
Charge Concentration, % : 61.5
Temperature, F : 68 ±2
Air Inlet Dew Point, F : 51 ±1
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : Variable
Air Flow Rate, Scfm : Variable
H_2 Flow Rate, Slpm : 0.30 ±0.02

FIGURE 7 EFFECT OF AIR FLOW RATE AT FOUR PCO_2 LEVELS



Test Number : 147C-4
Operating Time, Hr : 457.0
Number of Cells : 1
Current, Amp : Variable
Electrolyte : Cs_2CO_3
Charge Concentration, % : 61.5
Temperature, F : 68 ±2
Air Inlet Dew Point, F : 50 ±1
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : Variable
Air Flow Rate, Scfm : 0.44 ±0.02
H_2 Flow Rate, Slpm : 0.30 ±0.02

FIGURE 8 EFFECT OF LOW CURRENT DENSITY AND PCO_2

Test Number : 147C-4
Operating Time, Hr : 457.0
Number of Cells : 1
Current, Amp : Variable
Electrolyte : Cs_2CO_3
Charge Concentration, % : 61.5
Temperature, F : 68 ±2
Air Inlet Dew Point, F : 50 ±1
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : Variable
Air Flow Rate, Scfm : 0.44
H_2 Flow Rate, Slpm : 0.30 ±0.02

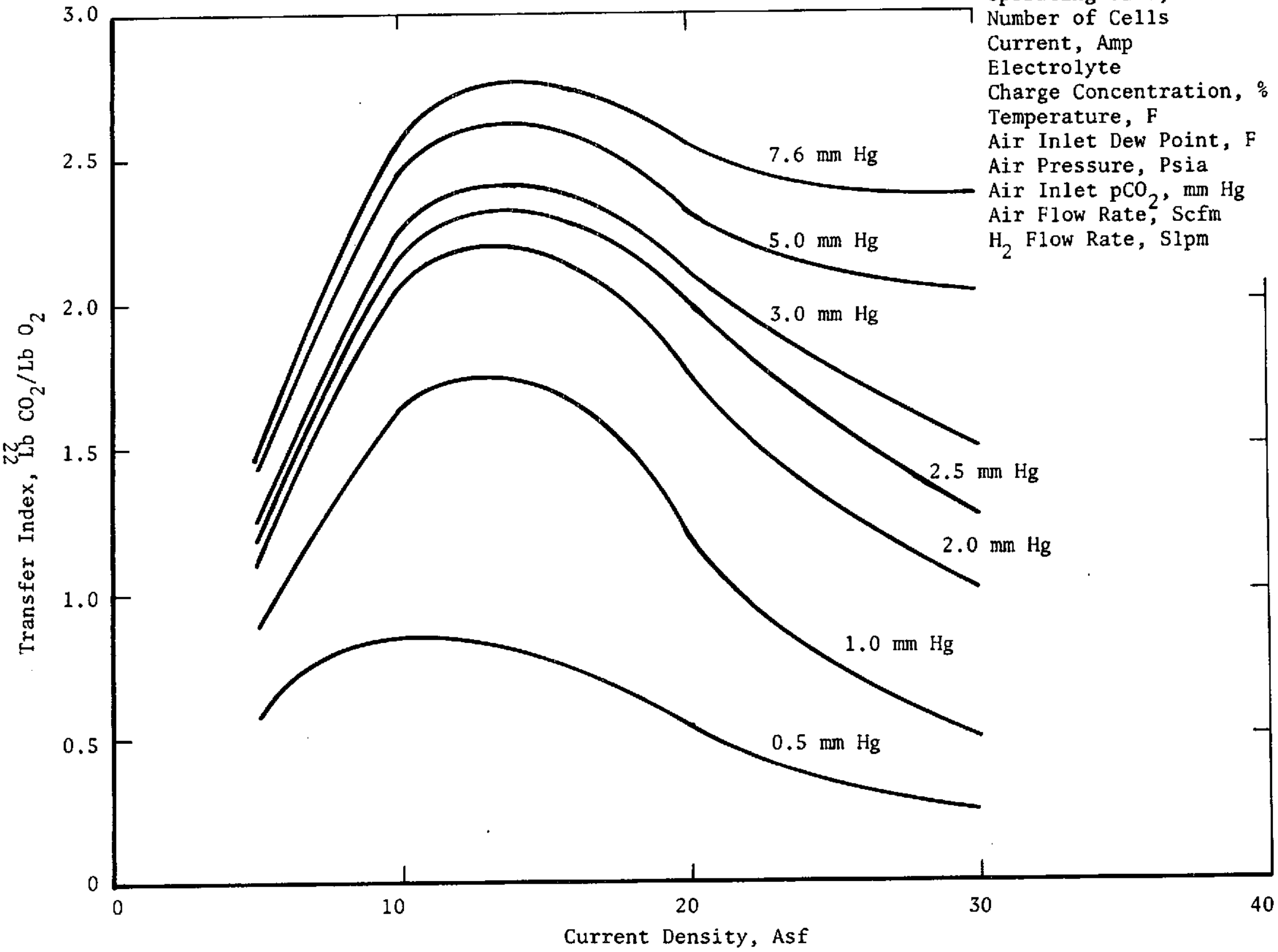


FIGURE 9 CROSSPLOT OF LOW CURRENT DENSITY CURVES

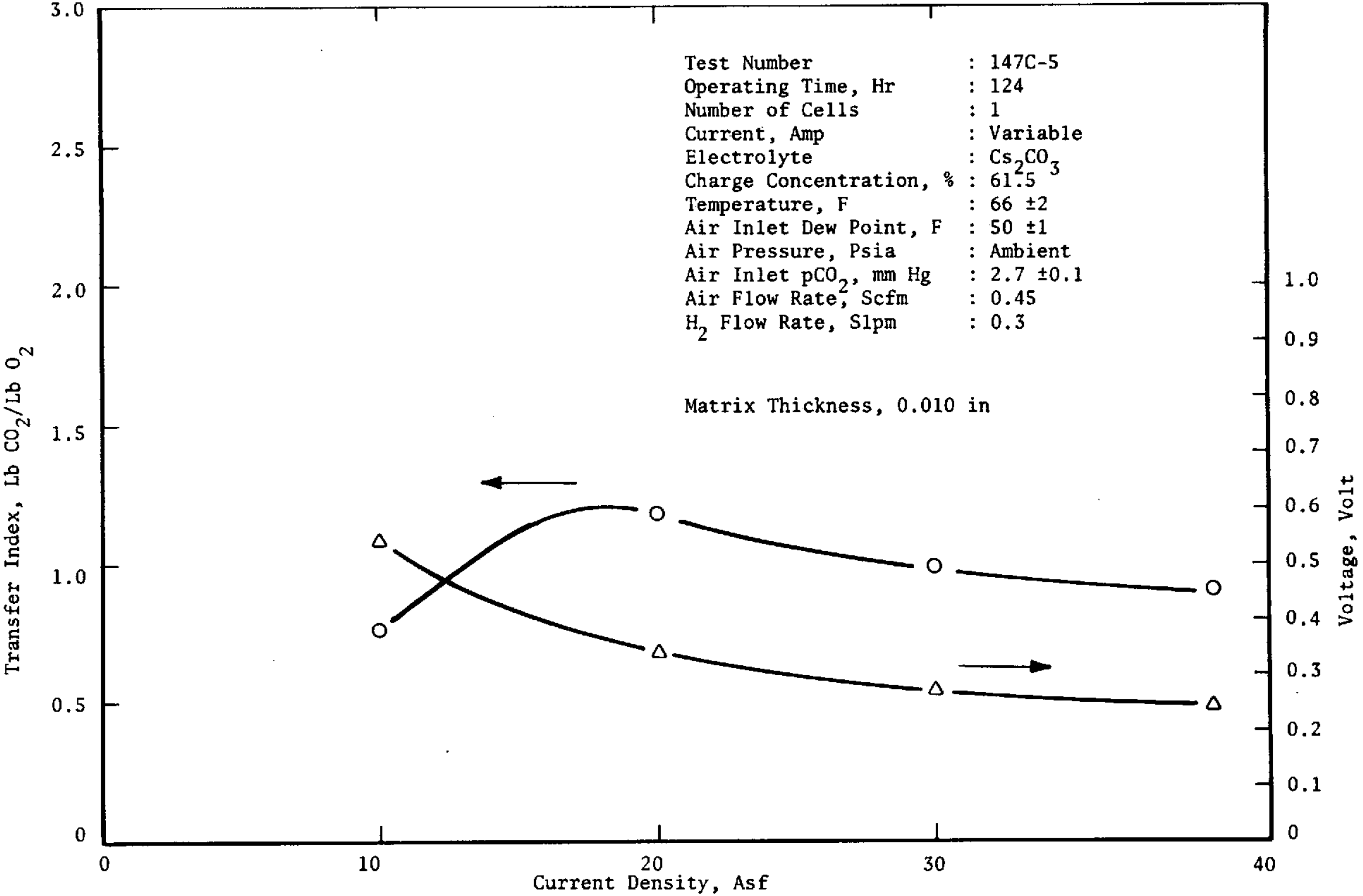


FIGURE 10 EFFECT OF MATRIX THICKNESS

(TI = 1.2 as opposed to 2.1 for the 0.030-inch baseline matrix) indicating that for the shorter diffusion length, cell concentration gradients were such that CO_2 backdiffusion inhibited CO_2 transfer. Cell voltage was not affected.

Effect of Electrode Thickness

EDC performance was determined as a function of current density for 0.005 inch thick electrodes, as opposed to the standard 0.010 inch thick electrodes used in Life Systems' EDC cell design. The results of the current density span are presented in Figure 11. The thinner electrodes increased TI from 2.1 for baseline configuration to 2.35. Cell voltage was unaffected. The increase in TI indicates that the electrode thickness improved air cavity convective mass transfer by decreasing the distance CO_2 has to diffuse through the electrode pores.

EDC Temperature Profile Determination (Thermal Gradient)

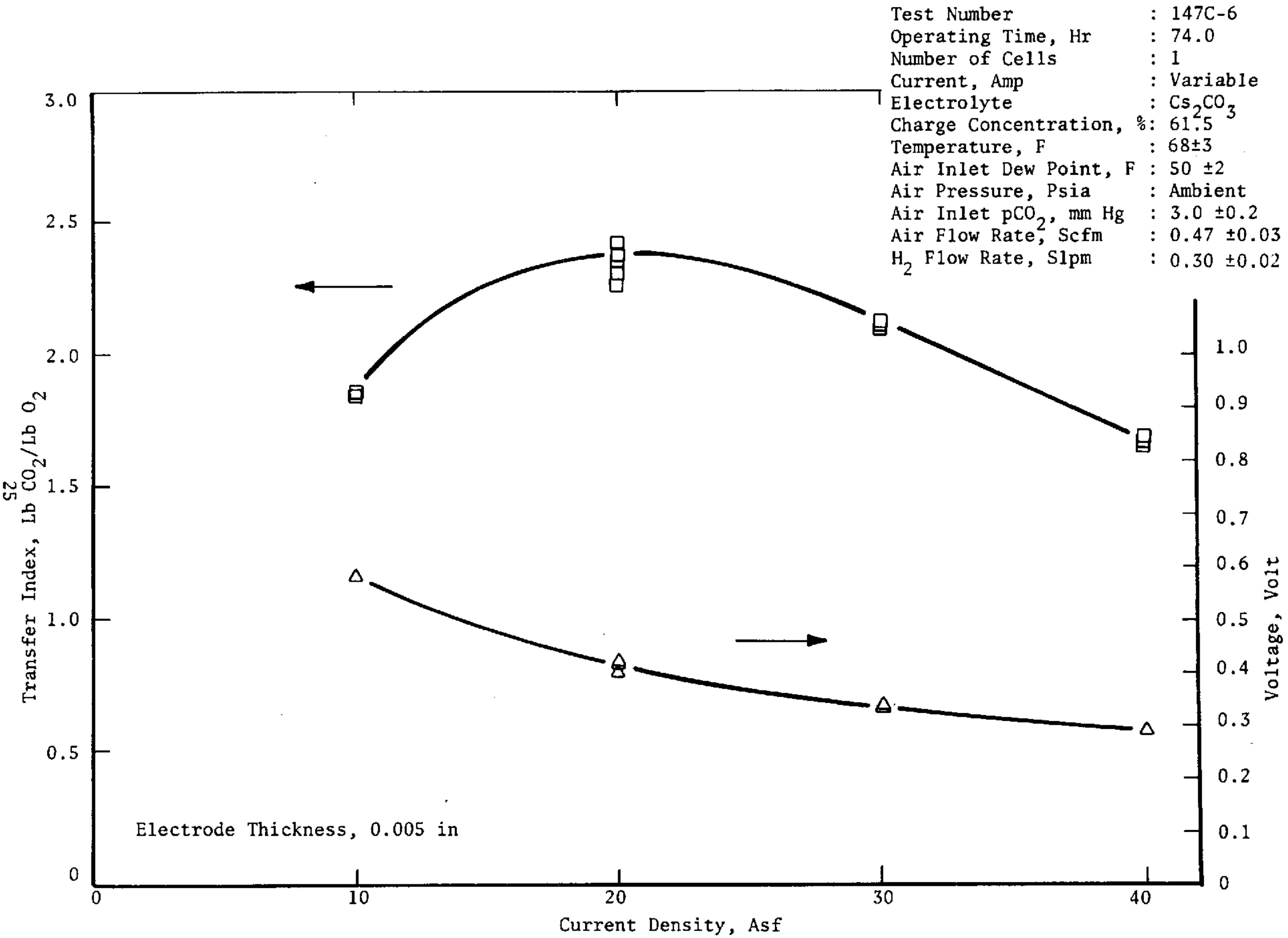
A temperature profile for an EDC cell was obtained for three process air heat load conditions: an air inlet relative humidity (RH) of 80% and 63% at 20 ASF and 80% at 40 ASF. Ten thermocouples were placed in the air cavity adjacent to, but not touching, the cathode. Two thermocouples were inserted, one each in the air inlet and air outlet manifolds. Two thermocouples were inserted in the cell matrix in the same plane as two air cavity thermocouples. The thermocouple location schematic is presented in Figure 12. The temperature profiles for the three process air heat load conditions are presented in Figures 13, 14 and 15. There was only a small difference in temperature between the thermocouples located in the cell matrix and those located in the air cavity. The air cavity temperature then reflects cell matrix temperature and can be used for moisture balance control.

Transient Response

EDC performance was measured as a function of time for step changes in current density, air flow rate and pCO_2. Step changes were made for one increase and one decrease in each of the three operating parameters and EDC performance was monitored as a function of time until equilibrium was reached. The transient responses in EDC performance for the six step changes are presented in Figures 16 through 21.

Transfer Index was measured on both the H_2 side and air side to determine transient differences in the CO_2 removed from the process air and concentrated into the process H_2. No transient differences were observed as the H_2 side and air side TI measurements agreed in experimental accuracy.

The step decrease in current density required the longest time for the EDC to regain equilibrium - 10 to 24 hours. The step increase in air flow required 3 to 4 hours for the EDC to regain equilibrium while both pCO_2 changes and the increase in current density and decrease in air flow required approximately 2 hours. Each cell voltage responded in 1 to 2 hours after a change in current density with only negligible effects being observed for the other parameter step changes.



Test Number : 147C-6
Operating Time, Hr : 74.0
Number of Cells : 1
Current, Amp : Variable
Electrolyte : Cs_2CO_3
Charge Concentration, %: 61.5
Temperature, F : 68±3
Air Inlet Dew Point, F : 50 ±2
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : 3.0 ±0.2
Air Flow Rate, Scfm : 0.47 ±0.03
H_2 Flow Rate, Slpm : 0.30 ±0.02

FIGURE 11 EFFECT OF ELECTRODE THICKNESS

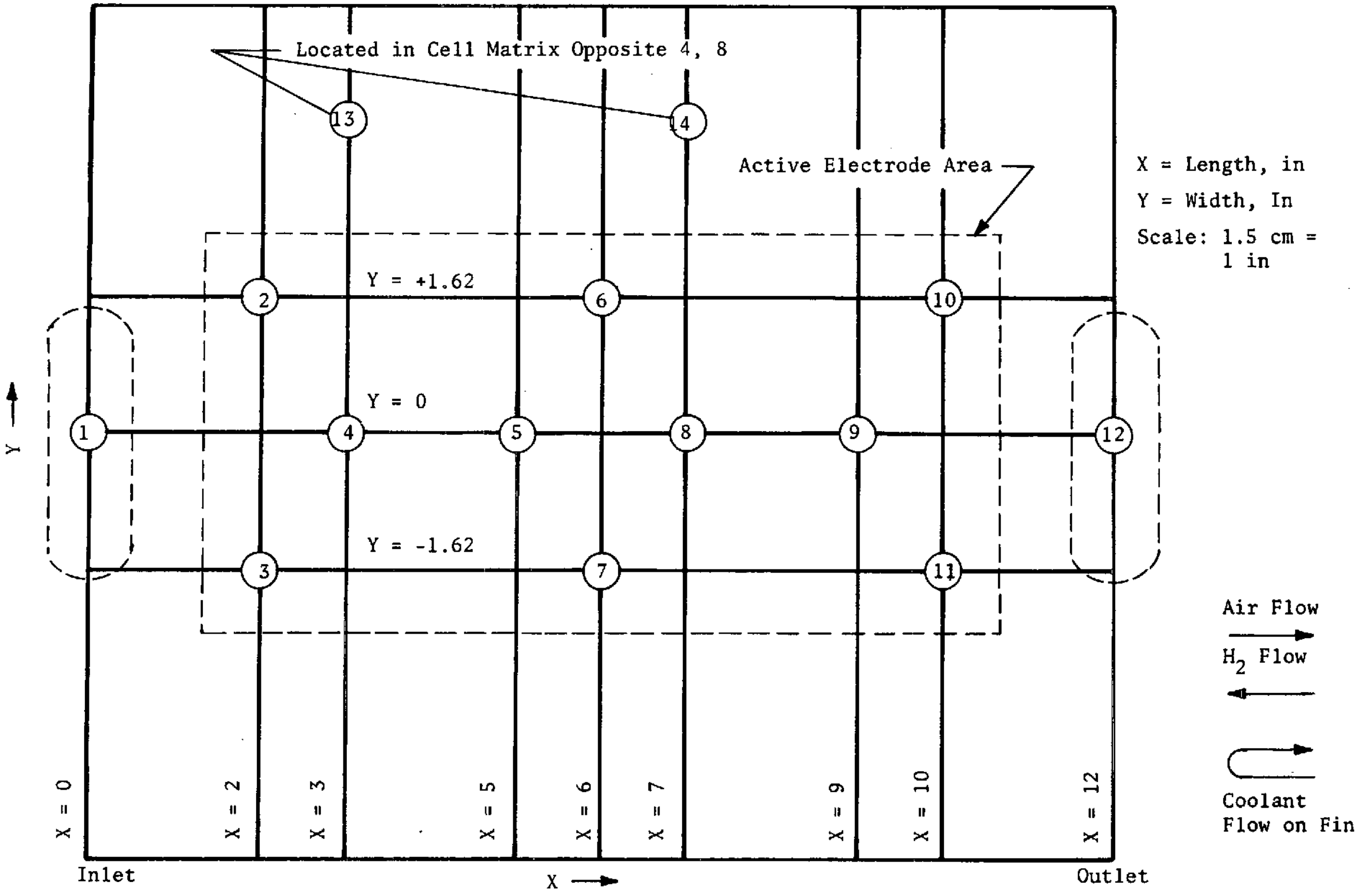
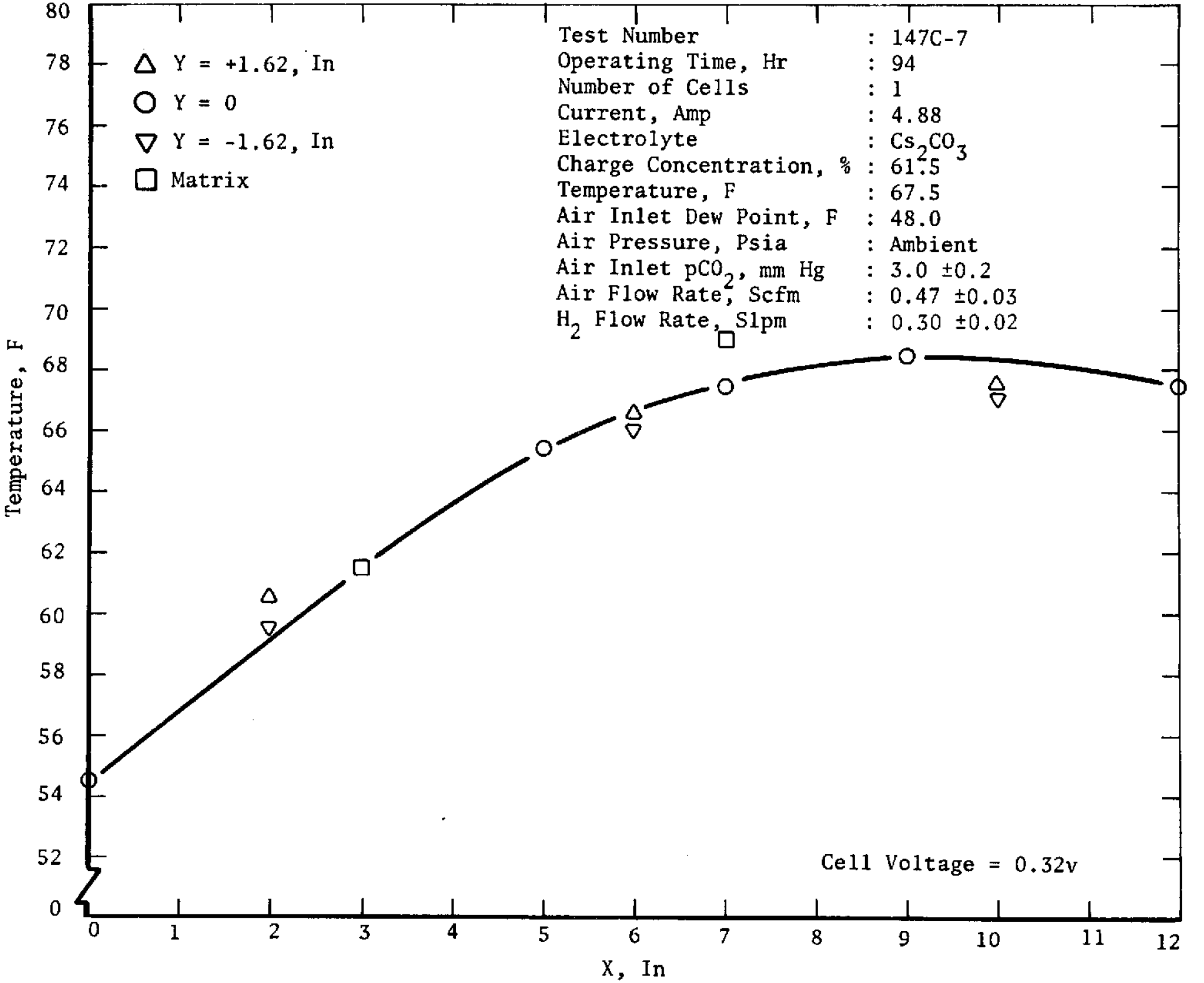
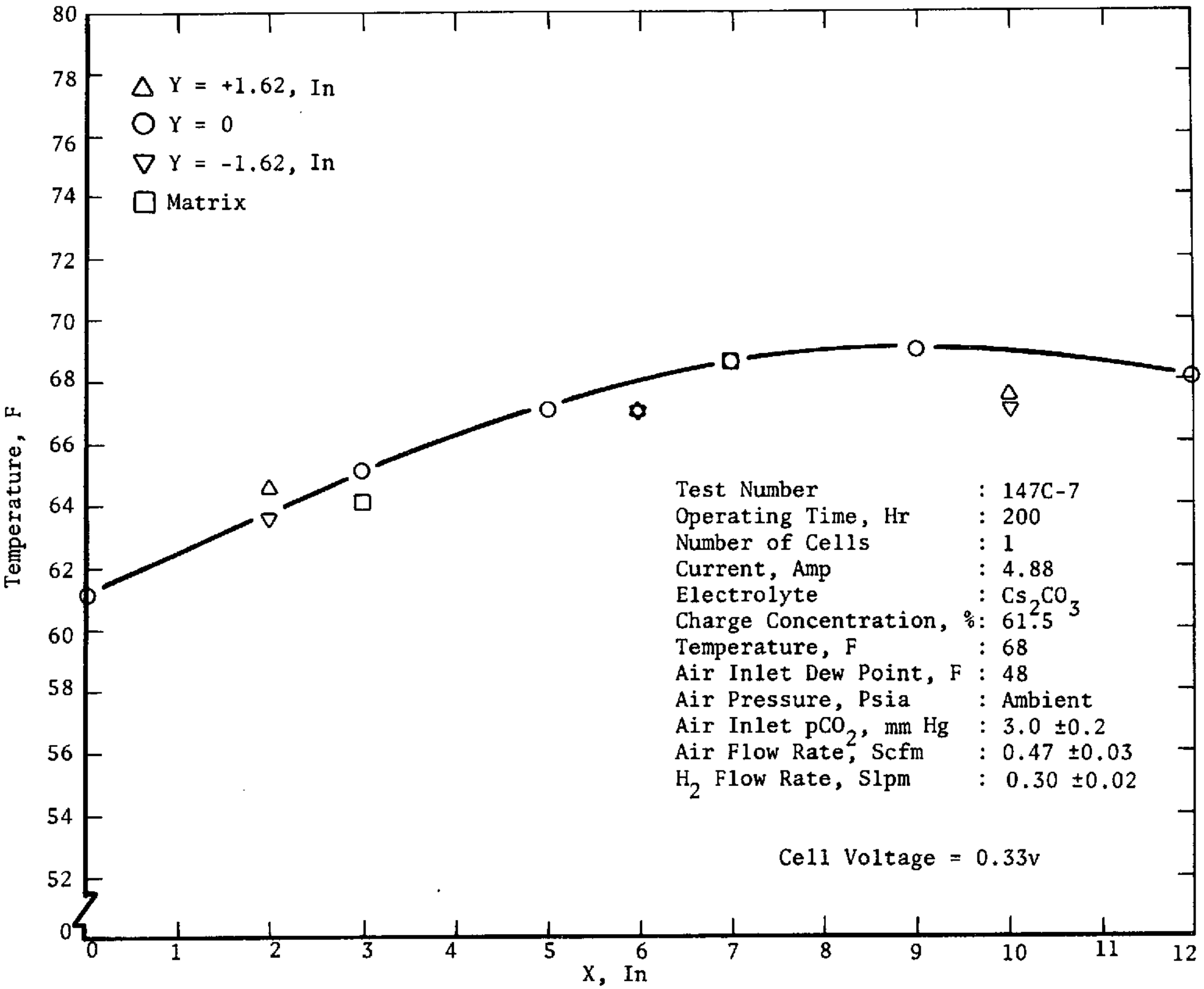


FIGURE 12 THERMOCOUPLE LOCATION SCHEMATIC



Test Number : 147C-7
Operating Time, Hr : 94
Number of Cells : 1
Current, Amp : 4.88
Electrolyte : Cs_2CO_3
Charge Concentration, % : 61.5
Temperature, F : 67.5
Air Inlet Dew Point, F : 48.0
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : 3.0 ±0.2
Air Flow Rate, Scfm : 0.47 ±0.03
H_2 Flow Rate, Slpm : 0.30 ±0.02

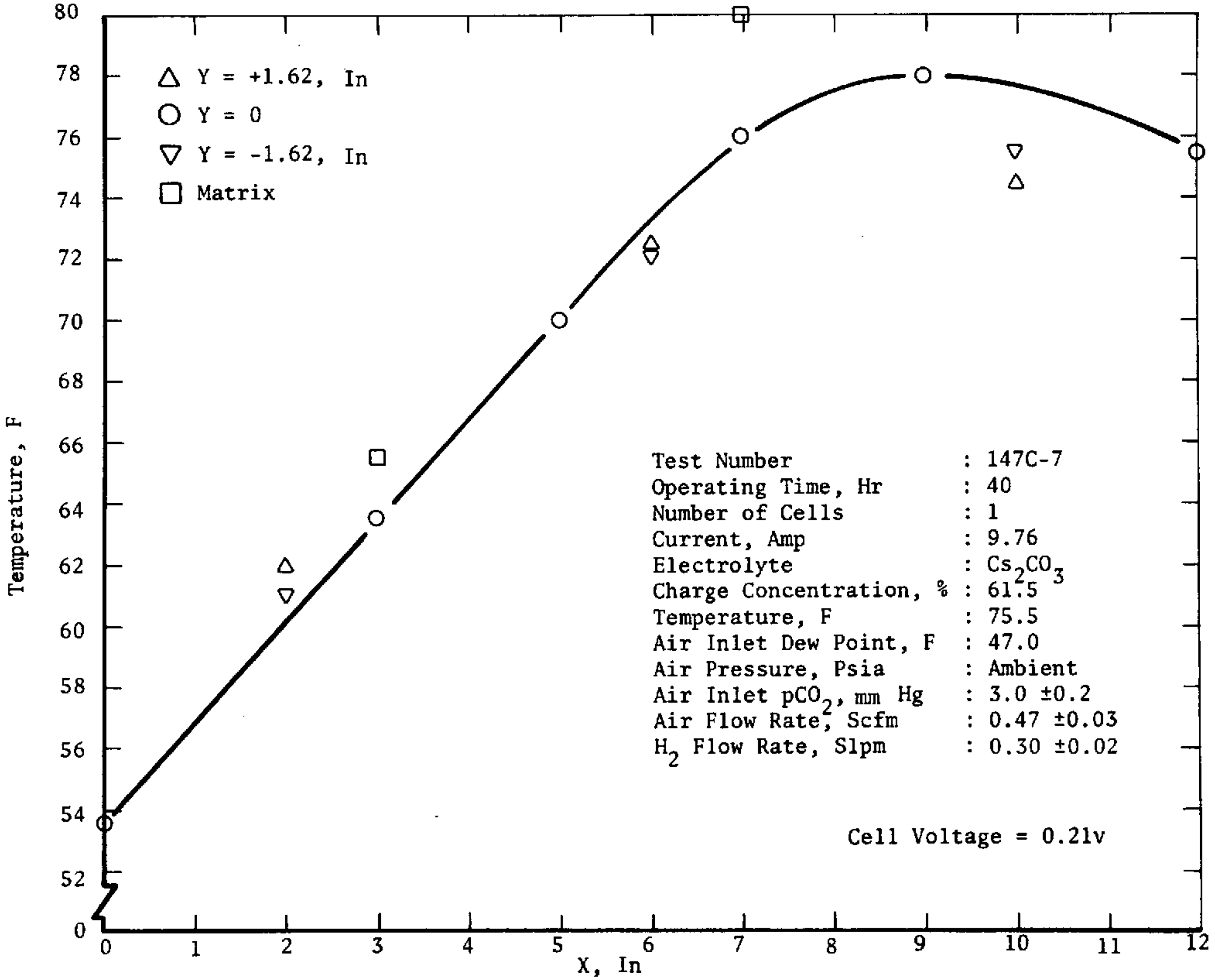
FIGURE 13 TEMPERATURE PROFILE FOR 80% AIR INLET RELATIVE HUMIDITY, 20 ASF



Test Number : 147C-7
Operating Time, Hr : 200
Number of Cells : 1
Current, Amp : 4.88
Electrolyte : Cs_2CO_3
Charge Concentration, %: 61.5
Temperature, F : 68
Air Inlet Dew Point, F : 48
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : 3.0 ±0.2
Air Flow Rate, Scfm : 0.47 ±0.03
H_2 Flow Rate, Slpm : 0.30 ±0.02

Cell Voltage = 0.33v

FIGURE 14 TEMPERATURE PROFILE FOR 63% AIR INLET RELATIVE HUMIDITY, 20 ASF



Test Number : 147C-7
Operating Time, Hr : 40
Number of Cells : 1
Current, Amp : 9.76
Electrolyte : Cs_2CO_3
Charge Concentration, % : 61.5
Temperature, F : 75.5
Air Inlet Dew Point, F : 47.0
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : 3.0 ±0.2
Air Flow Rate, Scfm : 0.47 ±0.03
H_2 Flow Rate, Slpm : 0.30 ±0.02

FIGURE 15 TEMPERATURE PROFILE FOR 80% AIR INLET RELATIVE HUMIDITY, 40 ASF

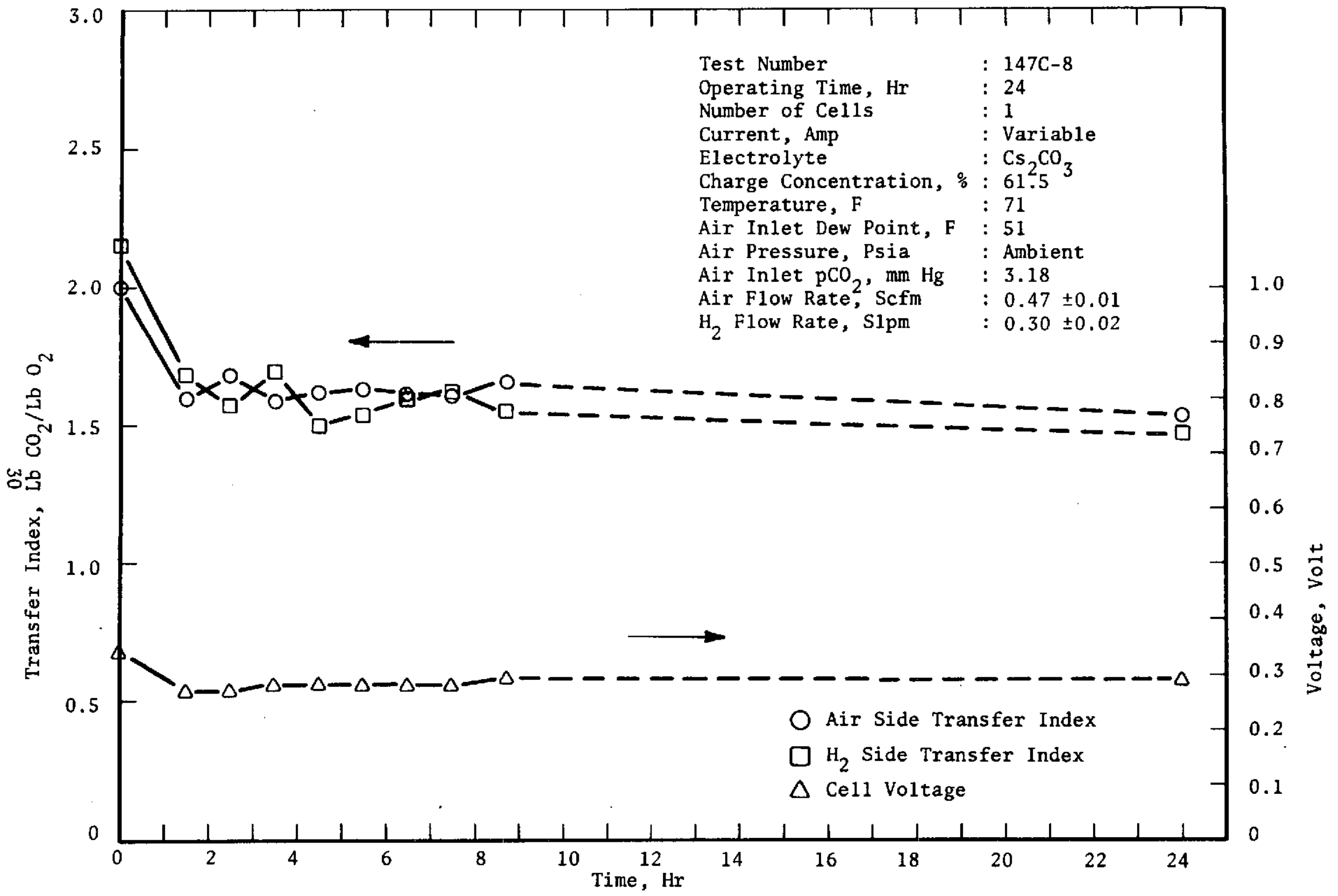
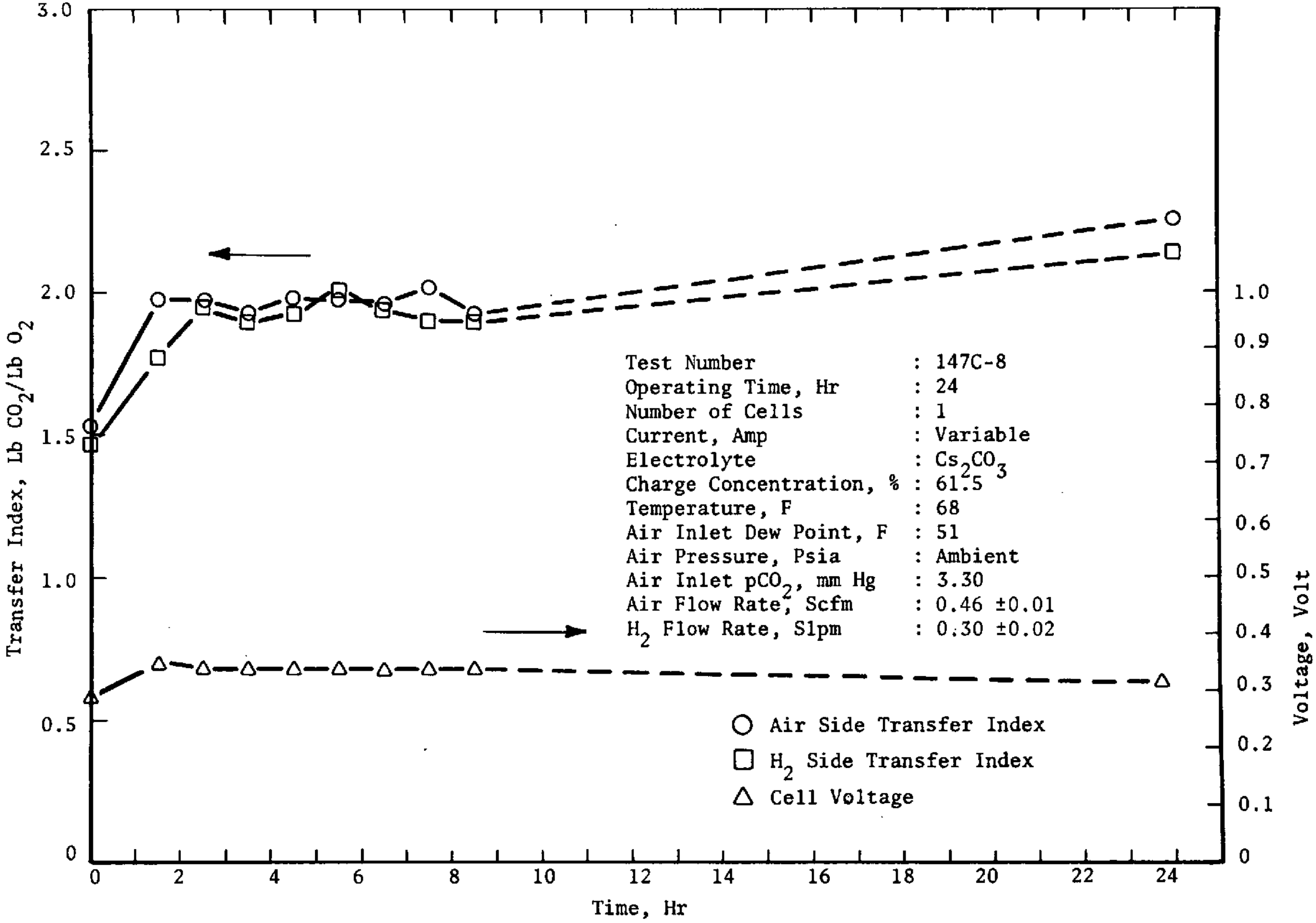
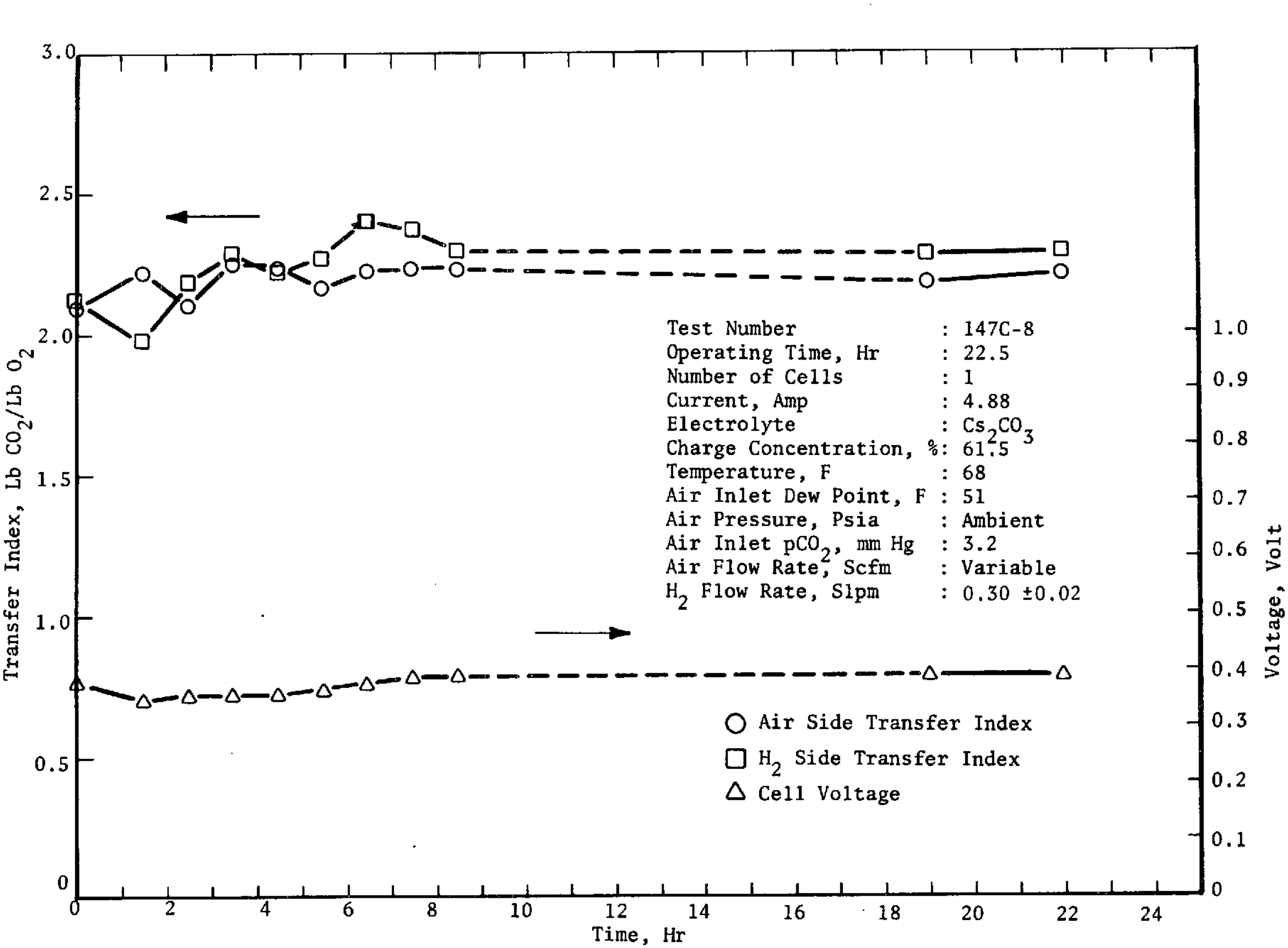


FIGURE 16 TRANSIENT RESPONSE OF A CO_2 CONCENTRATOR TO A STEP INCREASE IN CURRENT DENSITY (20 ASF TO 30 ASF)



Test Number : 147C-8
Operating Time, Hr : 24
Number of Cells : 1
Current, Amp : Variable
Electrolyte : Cs_2CO_3
Charge Concentration, % : 61.5
Temperature, F : 68
Air Inlet Dew Point, F : 51
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : 3.30
Air Flow Rate, Scfm : 0.46 ±0.01
H_2 Flow Rate, Slpm : 0.30 ±0.02

FIGURE 17 TRANSIENT RESPONSE OF A CO_2 CONCENTRATOR TO A STEP DECREASE IN CURRENT DENSITY (30 ASF TO 20 ASF)



Test Number : 147C-8
Operating Time, Hr : 22.5
Number of Cells : 1
Current, Amp : 4.88
Electrolyte : Cs_2CO_3
Charge Concentration, %: 61.5
Temperature, F : 68
Air Inlet Dew Point, F : 51
Air Pressure, Psia : Ambient
Air Inlet pCO_2, mm Hg : 3.2
Air Flow Rate, Scfm : Variable
H_2 Flow Rate, Slpm : 0.30 ±0.02

FIGURE 18 TRANSIENT RESPONSE OF A CO_2 CONCENTRATOR TO A STEP INCREASE IN AIR FLOW (0.48 SCFM TO 0.91 SCFM)

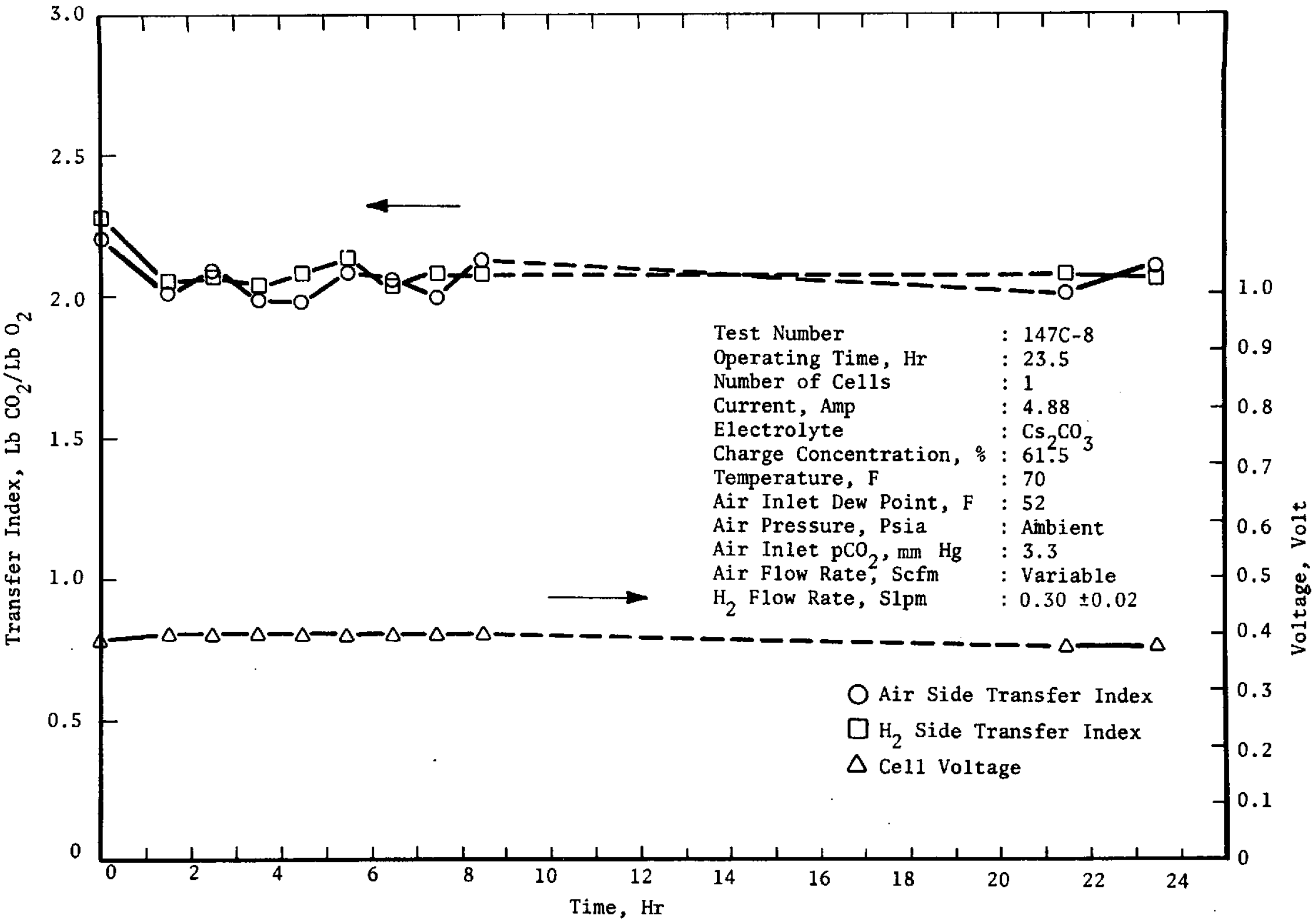


FIGURE 19 TRANSIENT RESPONSE OF A CO_2 CONCENTRATOR TO A STEP DECREASE IN AIR FLOW (0.91 SCFM TO 0.49 SCFM)

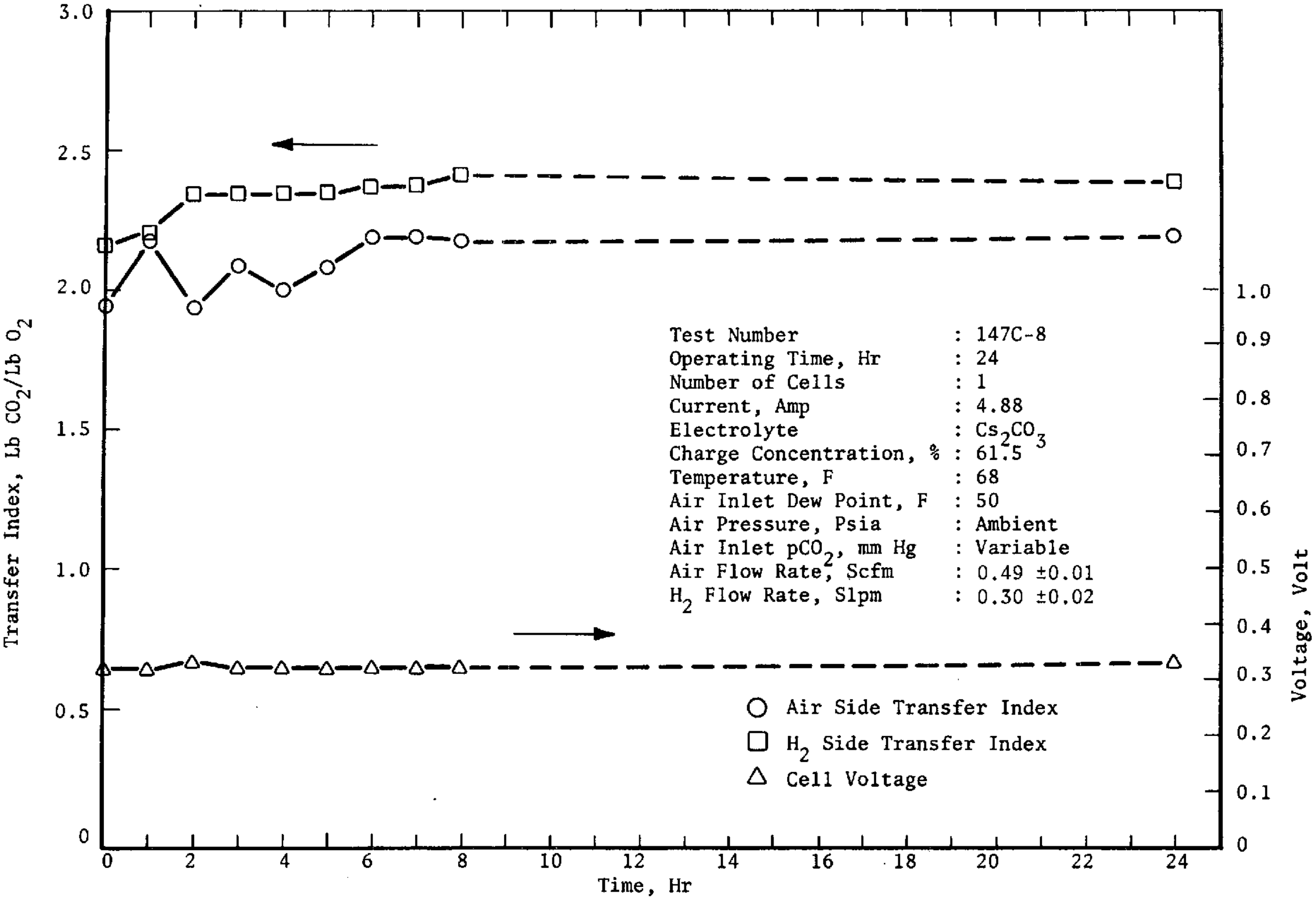


FIGURE 20 TRANSIENT RESPONSE OF A CO_2 CONCENTRATOR TO A STEP INCREASE IN INLET PCO_2 (3.0 MM HG TO 5.5 MM HG)

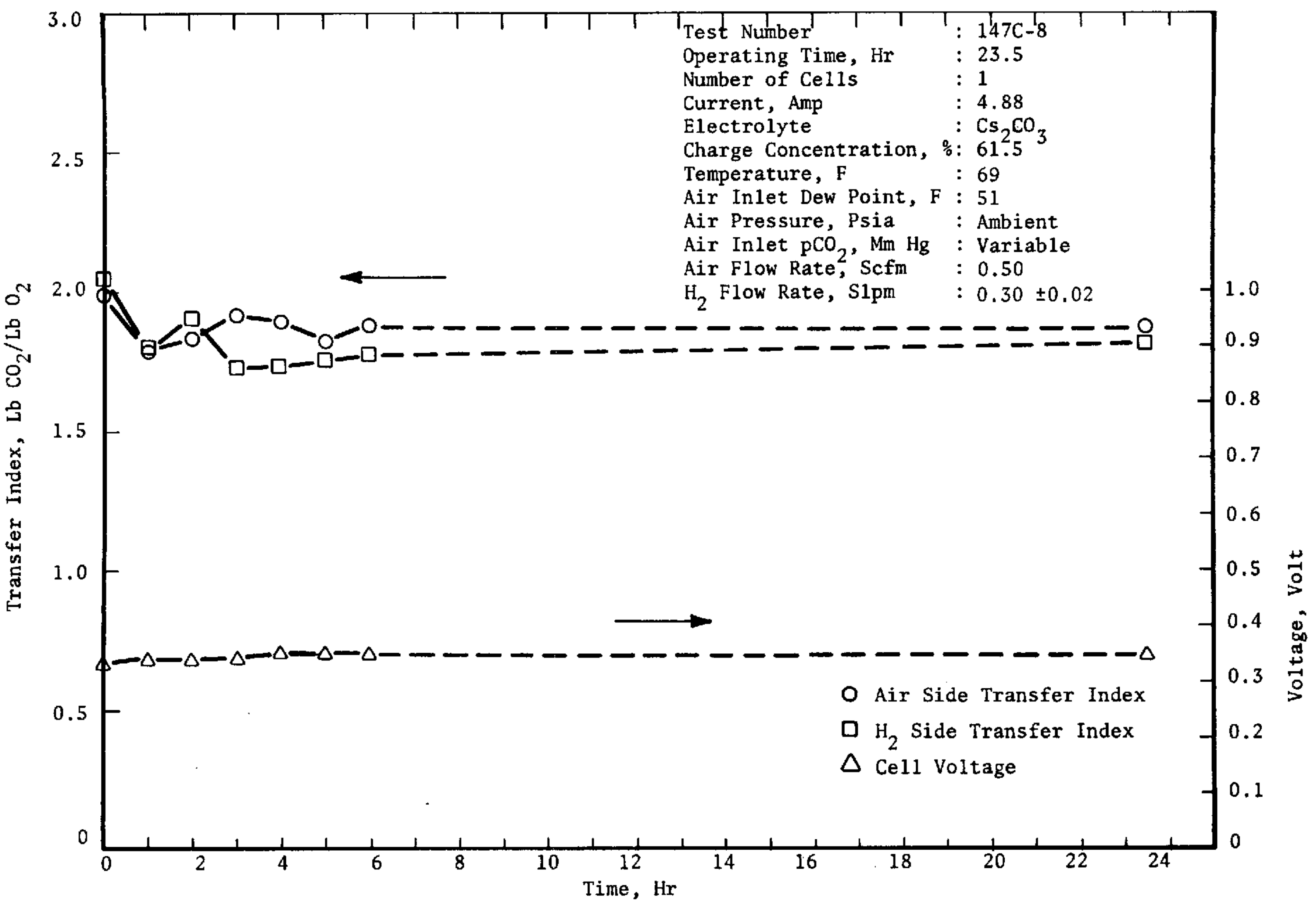


FIGURE 21 TRANSIENT RESPONSE OF A CO_2 CONCENTRATOR TO A STEP DECREASE IN INLET PCO_2 (5.0 MM HG TO 2.8 MM HG)

EMPIRICAL CORRELATIONS

Experimental results graphically define the interaction between the major operating parameters and EDC performance. These graphically defined relationships were transformed into empirical correlations or mathematical expressions for use in the computer simulation program.

Empirical correlations were required for the computer simulation model in four areas

1. CO_2 removal efficiency,
2. cell voltage,
3. moisture tolerance, and
4. heat removal.

CO_2 Removal Efficiency

The TI was experimentally found to be a function of process air inlet pCO_2, current density and process air flow rate as predicted by theory. A combination of the results obtained in the mathematical model experiments and data selected from previous tests on 1-, 3-, 15-, and 90-cell EDC designs yielded the set of data points shown in Figure 22. These data provided ithe basis for the empirical correlation for TI as a function of process air inlet pCO_2 and current density. A fifth-degree polynomial was fitted by the least-squares method through the data points obtained for 10, 20, 30 and 40 ASF. The equation used in the data fitting program was

$$TI = \sum_{i=1}^{5} S_i (pCO_2)^i$$

Where

S_i = the constants for a given current density.

Similar equations were added for 15, 25 and 35 ASF to aid in interpolating between curves. The values for S_i are given in Table 4. Simultation curves for 10, 20, 30 and 40 ASF drawn through the data points on Figure 22 verify prediction. As can be seen, the simulation curves obtained using the polynomial relationship describes the data within experimental error.

The effect of process air flow was incorporated into the TI correlation by using a normalized value for the inlet pCO_2 as a function of air flow rate. The correlation derived for the normalized pCO_2 was based on experimental results and is given by the following equation

$$P_a = pCO_2 \times (V/0.44)^{(0.45 - 0.0045\, pCO_2{}^2)}$$

Where

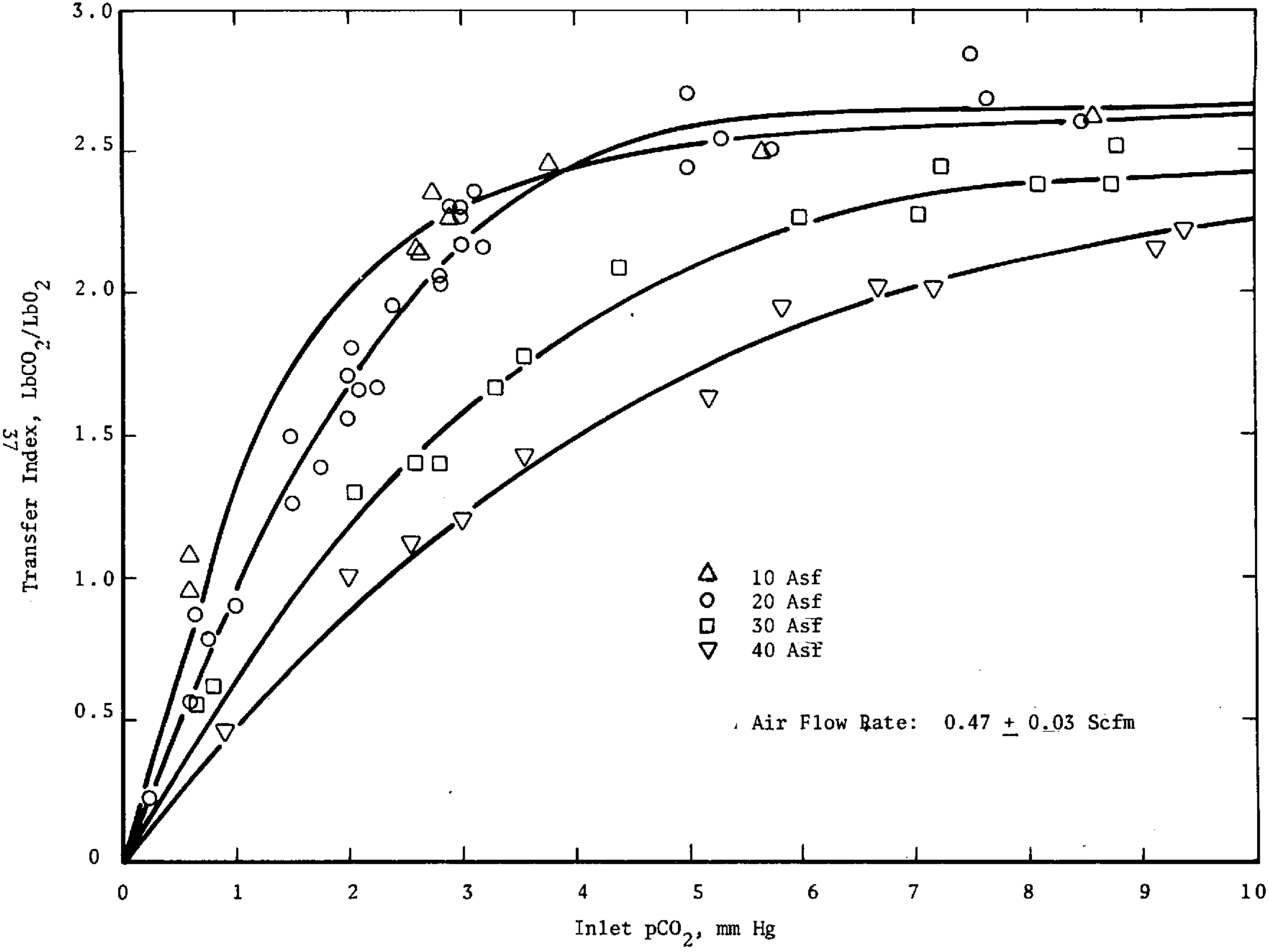


FIGURE 22 TI AS A FUNCTION OF pCO_2 AND CURRENT DENSITY

TABLE 4 VALUES FOR S_i CONSTANTS

Current Density Asf	S_1	S_2	S_3	S_4	S_5
10	1.75187	-5.11449×10^{-1}	7.75073×10^{-2}	-5.92584×10^{-3}	1.79862×10^{-4}
15	1.42306	-2.71935×10^{-1}	2.10187×10^{-2}	-3.4839×10^{-4}	-1.8475×10^{-5}
20	1.08190	-1.10821×10^{-1}	-8.1408×10^{-3}	1.96359×10^{-3}	-8.5832×10^{-5}
25	9.0258×10^{-1}	-1.05068×10^{-1}	2.5161×10^{-3}	2.8694×10^{-4}	-1.3673×10^{-5}
30	7.1551×10^{-1}	-7.2213×10^{-2}	2.4297×10^{-3}	9.08×10^{-6}	-3.48×10^{-7}
35	6.1612×10^{-1}	-5.5237×10^{-2}	3.803×10^{-4}	2.8605×10^{-4}	1.5623×10^{-5}
40	5.2087×10^{-1}	-3.5109×10^{-2}	-1.4939×10^{-3}	3.5115×10^{-4}	-1.4808×10^{-5}

P_a = corrected pCO_2, mm Hg

V = volumetric air flow rate, scfm

pCO_2 = process air inlet pCO_2, mm Hg

A comparison of experimental data and the simulation curves for TI as a function of process air flow rate at 20 ASF is presented in Figure 23.

Based on the two correlations for TI, a combined polynomial describing TI as a function of pCO_2 and process air flow rate at each current density can be written as

$$TI = S_{1,j}P_a + S_{2,j}P_a^2 + \ldots + S_{5,j}P_a^5$$

Where

j = 1 at 10 ASF, 2 at 15 ASF, ... and 7 at 40 ASF

Cell Voltage

As predicted by theory, experimental results show cell voltage was to be a function of current density and temperature. Data obtained for cell voltage as a function of current density (at 78F) were fitted to the general voltage current relationship as presented in the theoretical cell voltage discussion.

Cell voltage data obtained as a function of temperature were used to correct the voltage current correlation on temperature values other than 78F. The temperature correction was found to be a constant 5 mv/F. The resulting empirical voltage correlation is

$$E = 0.729 - 0.22 \ln I + 0.008\ I + 0.005\ (T-78)$$

Where

E = cell voltage, volt

I = cell current, amp

T = cell temperature, F

Figures 24 and 25 show the simulation curves and experimental data for cell voltage as a function of current density and temperature, respectively.

Moisture Tolerance

For proper EDC performance the cell must remain in moisture balance as previously defined. The computer simulation model must, therefore, insure that the operating conditions are within the cell moisture tolerance. In the actual operation of an EDC, the cell (air out) temperature is controlled at a set differential temperature above the process air inlet dew point temperature.

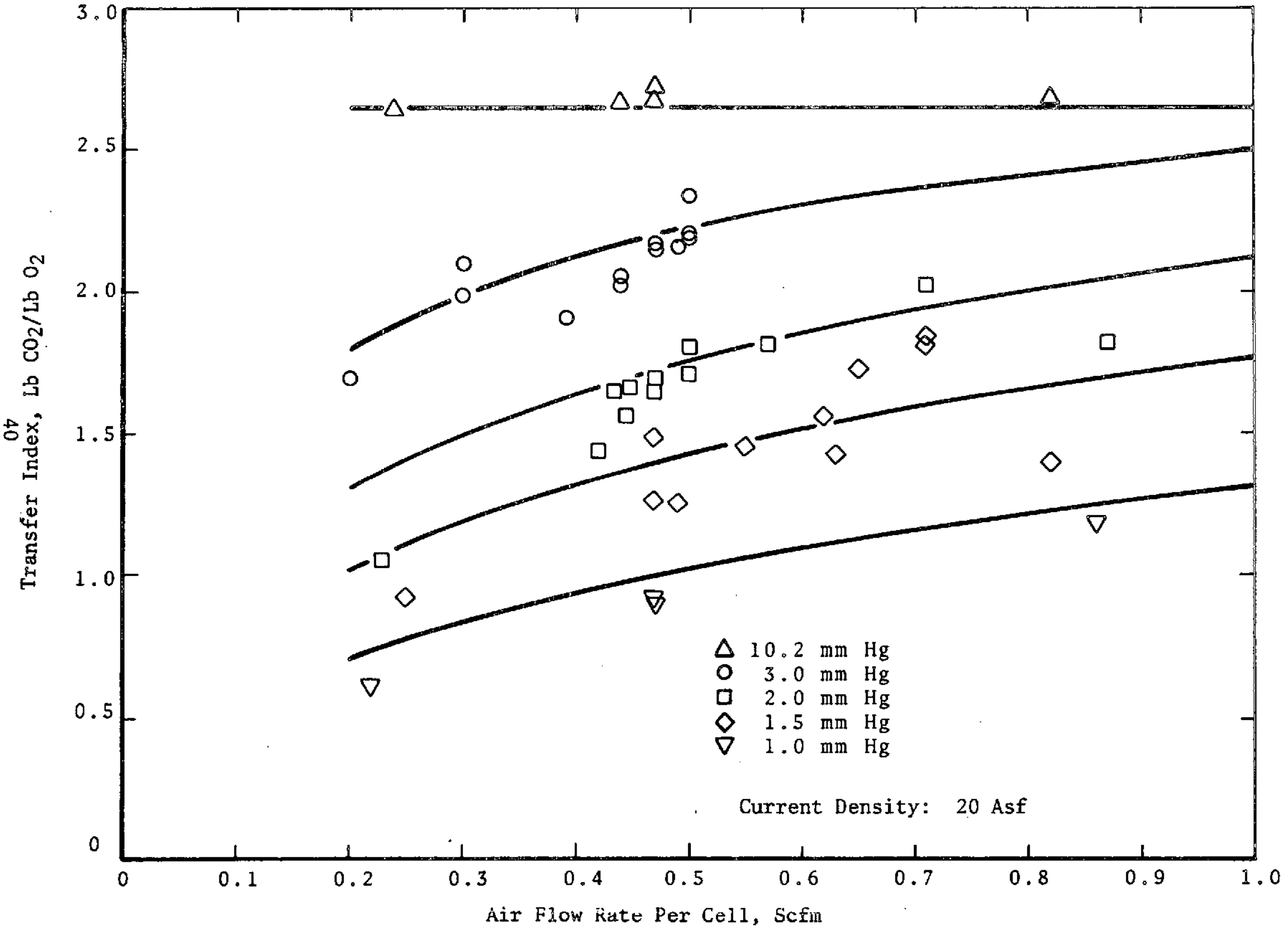


FIGURE 23 TI AS A FUNCTION OF AIR FLOW RATE AND PCO_2

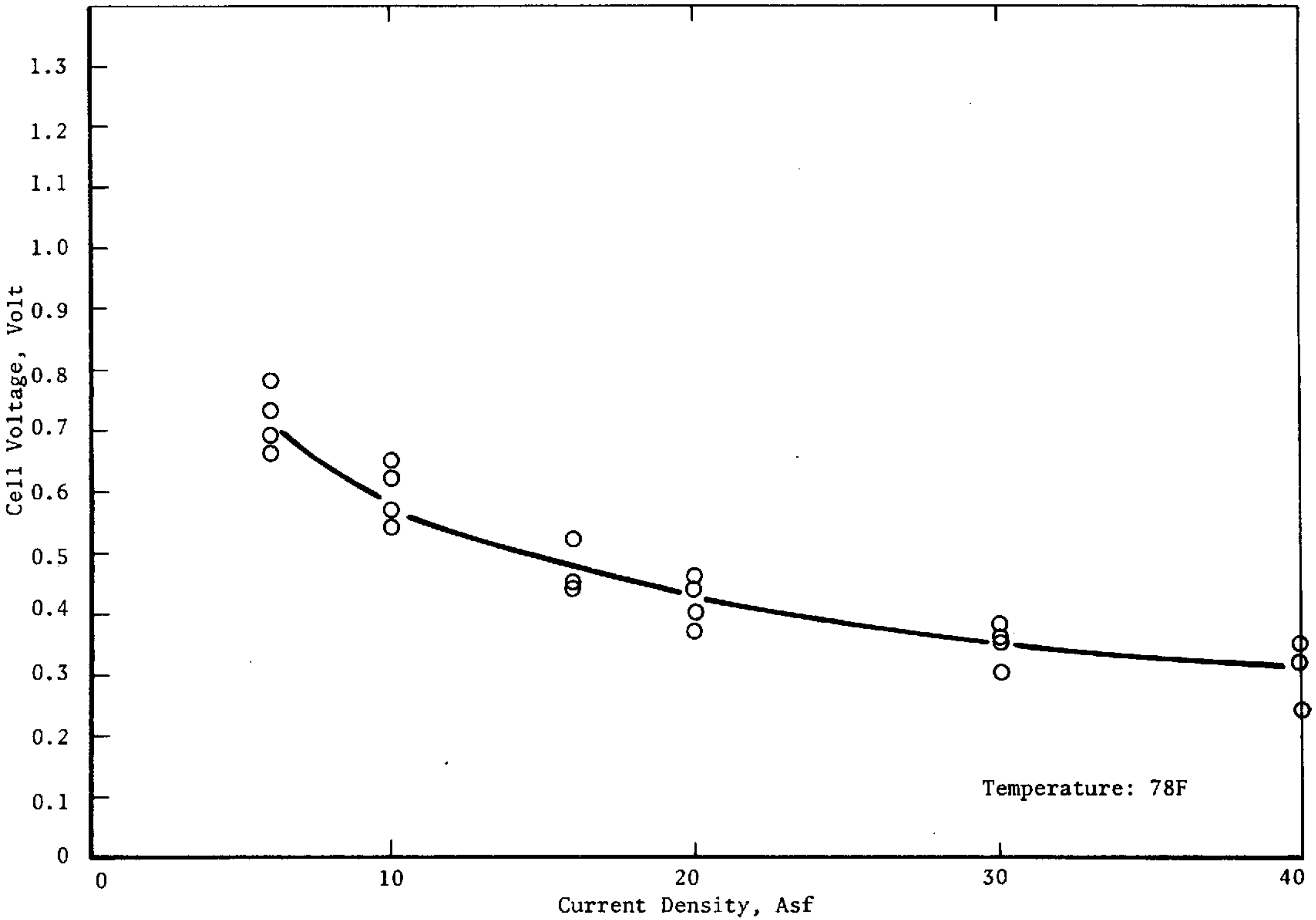


FIGURE 24 CELL VOLTAGE AS A FUNCTION OF CURRENT DENSITY

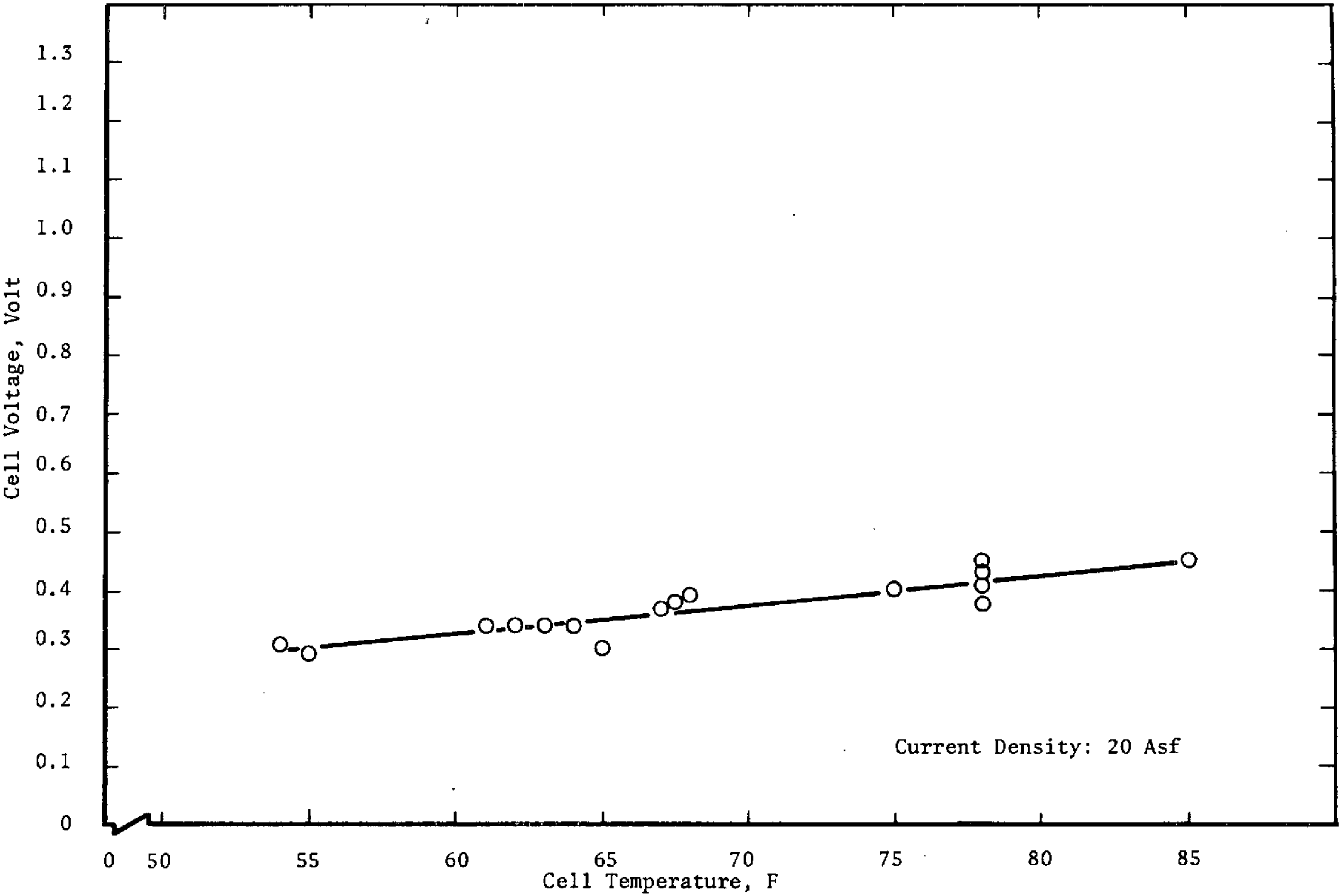


FIGURE 25 CELL VOLTAGE AS A FUNCTION OF TEMPERATURE

The temperature difference is controlled at a value determined by the nominal range in process air humidity conditions and current density (H_2O production).

Once the magnitude of the temperature differential is set, the cell temperature control scheme will maintain moisture balance based on the incoming process air humidity conditions. Should humidity conditions fall outside the nominal range, the cell temperature control scheme may be unable to maintain cell moisture in balance.

The moisture tolerance of a cell initially charged with 61.5 ± 0.5% w/w Cs_2CO_3 at current densities between 10 and 40 ASF has been determined experimentally to be given by the following set of conditions.

1. $9.5 \le T_1 - DP_1 \le 13$ and $9.5 \le T_2 - DP_2 \le 13$
2. $4 \le T_1 - DP_1 \le 14$, $7 \le T_2 - DP_2 \le 19$, $9.5 \le (T_1 - DP_1 + T_2 - DP_2)/2$

and either

$$13 \le T_2 - DP_2$$

or

$$10 \le (T_1 - DP_1 + T_2 - DP_2)/2$$

Where

T = process air inlet temperature, F

DP_1 = process air inlet dew point, F

T_2 = process air outlet temperature, F

DP_2 = process air outlet dew point, F

One of the two conditions must be met to maintain moisture balance. These conditions are shown graphically in Figure 26.

Heat Removal

For the computer simulation, it is assumed that there is sufficient heat removal capacity in the cooling air (flow rate and temperature) to maintain cell temperature (and, hence, moisture balance) at the required level. For a given cooling air temperature, the cooling air flow rate required to maintain cell temperature must be calculated. Two correlations are required for this calculation: the convective heat transfer coefficient and the cooling fin efficiency. The correlations used were obtained from data presented in literature.(6) For the geometry of the cell cooling fins attached to the anode current collector, the convective heat transfer coefficient is assumed to be a function of the cooling air flow rate only. The following correlation was used for the convective heat transfer coefficient in a rectangular channel.

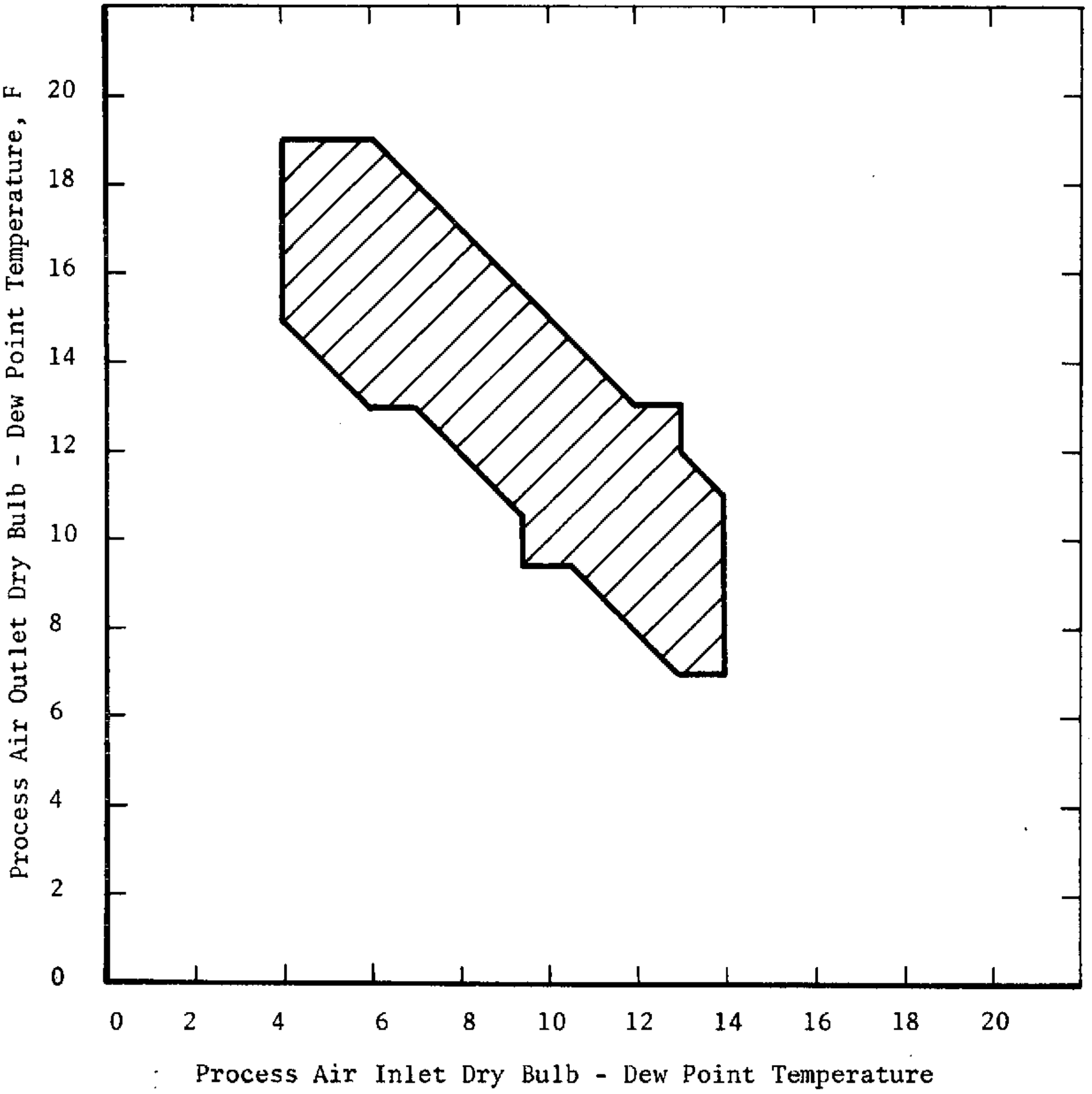


FIGURE 26 EDC MOISTURE TOLERANCE

If $V \leq 1$, $h = 1.97V^{0.3333}$

If $1<V<2.9883$, $h = 1.21 + 0.34 + 0.42V^2$

If $2.9883 \leq V \leq 4$, $h = 2V$

If $4<V$, $h = 2.639016V^{0.8}$

Where

V = cooling air flow rate per cell, scfm

h = convective heat transfer coefficient, Btu/hr-F-ft^2

The following formula was used to calculate the fin efficiency

If $V<0.32194$, $\eta= 1$

If $0.32194 <V<24.72$, $\eta= 1.0744 - 0.1135V^{0.5}$

If $24.72 <V$, $\eta= 2.486V^{-0.5}$

COMPUTER SIMULATION MODEL

The computer simulation model uses the empirical correlations obtained for TI, cell voltage, moisture tolerance, and heat removal to describe EDC performance and solve EDC heat and mass balance equations as a function of 14 input parameters. Figure 27 is a block diagram of an EDC showing the six process streams entering and exiting an EDC module. The 14 input variables, or parameters, describe the inlet process streams and module-operating parameters. The ranges in the input variables over which the simulation model can predict accurately EDC performance are given in Table 5.

Model Analysis

The simulation model completes the description of the process air and H_2 streams by calculating component flow rates and partial pressures. The vapor pressure and relative humidity of each stream is calculated from the dew point temperature using a correlation obtained from the literature.(7) Cell temperature is calculated from the process air inlet dew point temperature and DELT1. The TI and cell voltage correlation were solved and the results were used to calculate module performance parameters.

Cooling air flow rate is determined by calculating the temperature differential between the cell and cooling air temperatures required to remove the waste heat generated. The available temperature drop is assumed to be the log mean average temperature differential between the cell temperature and the cooling air inlet and outlet temperatures. Cooling air flow rate is then calculated by an iterative alogorithm such that ΔT required and ΔT available are within ±0.001 F.

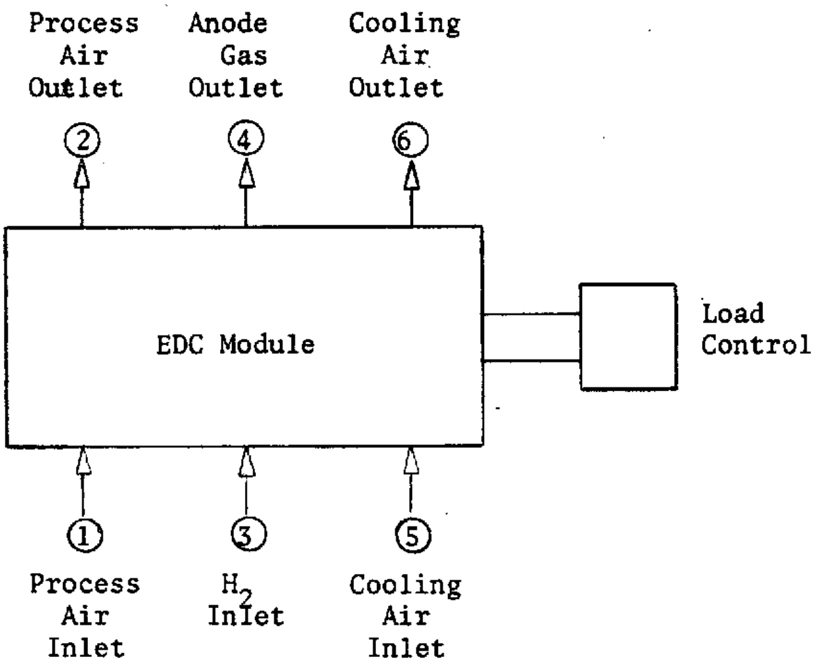


FIGURE 27 EDC BLOCK DIAGRAM

TABLE 5 INPUT VARIABLE RANGES

Process Air Inlet	
pCO_2	0.5-10 mm Hg
pO_2	2-4 Psia
Total Pressure	14.7 Psia
Dew Point Temperature	41-70F
Dry Bulb Temperature	47-80F
Flow Rate	0.2-0.8 Scfm/Cell(a)
Process H_2 Inlet	
Flow Rate	$\geq$1.3 x Stoichiometric
Dew Point Temperature	10-40F
Dry Bulb Temperature	65-75F
Pressure	0-5 Psig
Module	
Number of Cells	1-90
Current	2.44-9.76 Amp
DELT1(b)	15-25F
Cooling Air Inlet	
Temperature	$\leq$Process Air Inlet

(a) 70F and 14.7 Psia

(b) DELT1 = (Module Temperature - Process Air Inlet Dew Point)

Mass balances for CO_2, O_2, H_2 and H_2O are used to calculate the process outlet stream properties. The H_2 dew point out is assumed to be the average of the process air inlet and outlet dew points. A complete list of input and output variables is given in Table 6.

Computer Program

The computer program was written in Fortran IV for a Univac 1108 Digital Computer. Figure 28 is the flow chart for the computer program. The program line numbers are referenced above each step in the flow chart. The subroutine flow charts for calculating TI, cell voltage, dew points, H_2O vapor pressure and the solution of root functions are given in Figure 29. A listing of the computer program is given in Appendix C.

The program provides checks to insure that

1. there is a $\geq$1.3 x stoichiometric-in-current H_2 flow,
2. process air humidity conditions are within cell moisture tolerance, and
3. cooling air temperature is low enough and sufficient heat is generated to control module temperature.

Model Results

Emphasis was placed on the empirical correlations used in the computer program which resulted in the final simulation curves (shown as the solid lines) presented in Figures 22 through 26. Several sample outputs showing all calculated variables and the program variable checks are presented in Appendix D.

CONCLUSIONS

The following conclusions were reached as a direct result of mathematical model activities.

1. An EDC computer simulation model based on experimental results has been developed to predict EDC performance as a function of the input operating parameters for LSI's baseline cell configuration.
2. The simulation model can be used for integration studies when interfacing the EDC with other regenerative life support subsystems.
3. The computer model can be used to optimize performance as a function of the input conditions for the cell design modeled.
4. TI can be assumed to be a function of process air inlet pCO_2, current density and process air flow rate over normal EDC operating ranges.

TABLE 6 MATH MODEL INPUT AND OUTPUT VARIABLES

Input Variables

Process Air:	Inlet pCO_2, mm Hg
	Inlet pO_2, Psia
	Pressure, Psia
	Inlet Dry Bulb Temperature, F
	Inlet Dew Point Temperature, F
	Inlet Flow Rate, Scfm
Process H_2:	Inlet Flow Rate, Slpm
	Inlet Dry Bulb Temperature, F
	Inlet Dew Point, F
	Pressure, Psig
Module:	Number of Cells
	Current, Amps
	DELT1, F
Cooling Air:	Inlet Temperature, F

Output Variables

Module:	Temperature, F
	Cell Voltage, Volt
	Stack Voltage, Volt
	Current Density, Asf
	Power Output, Watt
	Heat Load, Btu/Hr
	O_2 Consumption, Lb/Hr
	H_2 Consumption, Lb/Hr
	H_2O Production, Lb/Hr
	Transfer Index, Lb CO_2/Lb O_2
	Transfer Efficiency, %
	CO_2 Removal Rate, Lb/Hr
	Preferred Value of DELT1, F
Process Air Inlet:	pCO_2, mm Hg
	Total Pressure, mm Hg
	pH_2O, mm Hg
	pN_2, mm Hg
	H_2O Flow Rate, Lb/Hr
	CO_2 Flow Rate, Lb/Hr
	Relative Humidity, %
	O_2 Flow Rate, Scfm
	H_2O Flow Rate, Scfm

Table 6 - Continued

Process Air Outlet:	Total Pressure, mm Hg
	pCO_2, mm Hg
	pH_2O, mm Hg
	Total Flow Rate, Scfm
	CO_2 Flow Rate, Scfm
	H_2O Flow Rate, Scfm
	N_2 Flow Rate, Scfm
	O_2 Flow Rate, Scfm
	CO_2 Flow Rate, Lb/Hr
	H_2O Flow Rate, Lb/Hr
	Dew Point Temperature, F
	Relative Humidity, %
Process H_2 Inlet:	Total Flow Rate, Scfm
	pH_2O, mm Hg
	Total Pressure, mm Hg
	pH_2, mm Hg
	H_2O Flow Rate, Scfm
	H_2 Flow Rate, Scfm
	H_2 Flow Rate, Lb/Hr
Anode Gas Outlet:	Dew Point Temperature, F
	pH_2O, mm Hg
	CO_2 Flow Rate, Lb/Hr
	H_2 Flow Rate, Scfm
	CO_2 Flow Rate, Scfm
	Total Pressure, mm Hg
	H_2O Flow Rate, Scfm
	H_2O Flow Rate, Lb/Hr
	Total Flow Rate, Scfm
	Total Flow Rate, Slpm
	H_2O Flow Rate, Slpm
	CO_2 Flow Rate, Slpm
	H_2 Flow Rate, Lb/Hr
	Total Flow Rate, Lb/Hr
	CO_2-H_2 Weight Ratio, Lb CO_2/Lb H_2
	H_2-CO_2 Volume Ratio, Ft^3 H_2/Ft^3 CO_2
Heat Balance:	Process Air Heat Pick-up, Btu/Hr
	Process H_2 Heat Pick-up, Btu/Hr
	Cooling Air Heat Pick-up, Btu/Hr
Cooling Air:	Flow Rate, Scfm
	Inlet Temperature, F
	Outlet Temperature, F
	Fin Convective Heat Transfer Coefficient, Btu Hr^{-1} Ft^{-2} F^{-1}
	Fin Efficiency, Fraction of Unity

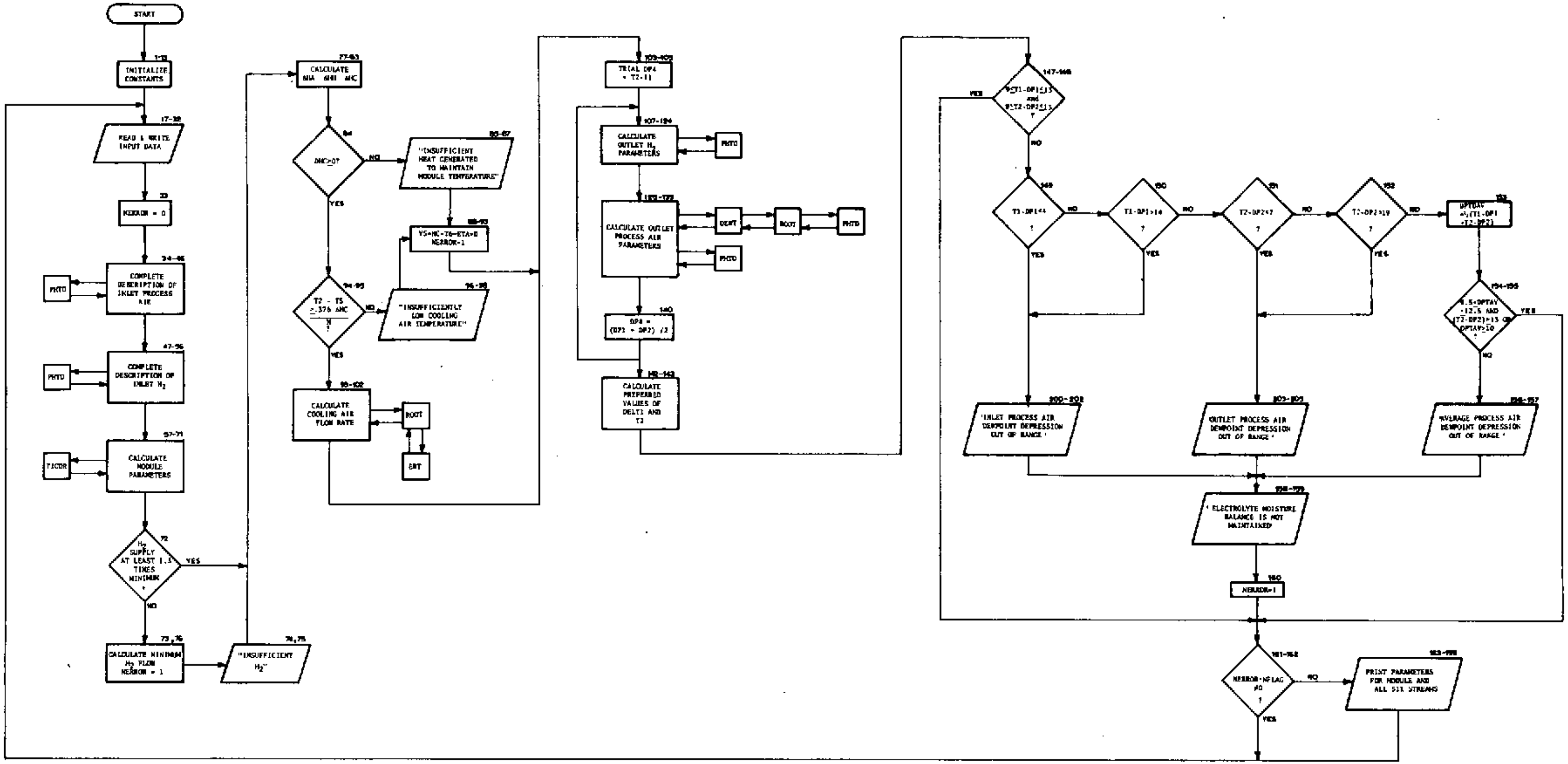


FIGURE 28 COMPUTER PROGRAM FLOW CHART

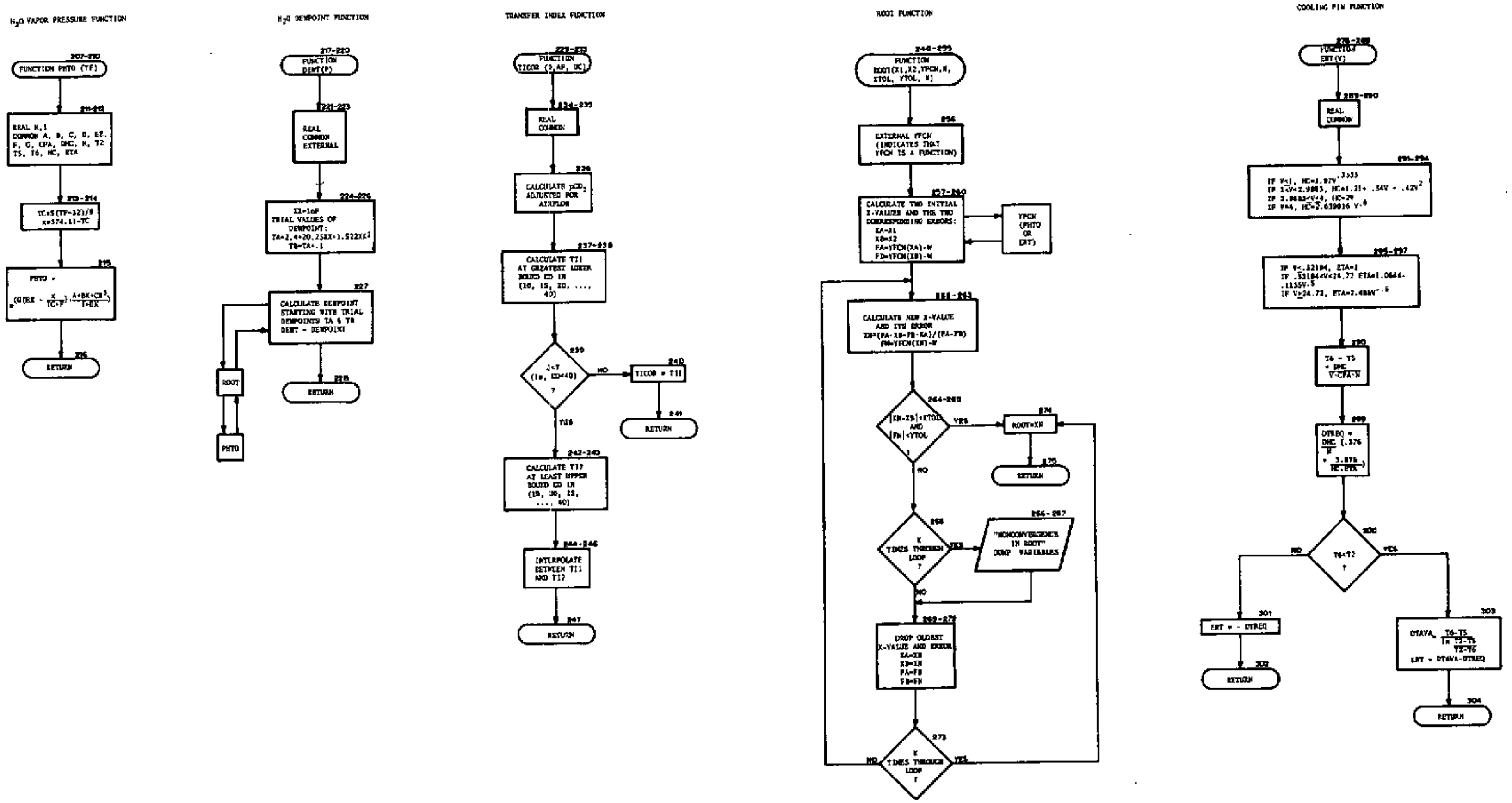


FIGURE 29 SUBROUTINES FLOW CHART

5. Series flow of H_2 to a 15-cell stack does not influence transfer efficiency or cell voltage for anode gas pCO_2 levels <640 mm Hg.

6. The formation factor for the cell electrolyte-filled matrix was found to be 6.0 ±0.2.

7. The mathematical model computer program should be expanded to include all components of an Electrochemical CO_2 Collection Subsystem and subsystem control schemes to enable total subsystem characterization and integration (by simulation model) with other spacecraft life support subsystems.

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APPENDIX A FORMATION FACTOR CALCULATIONS

The formation factor is defined by the equation

$$f = R_v/R_o$$

Where

f = formation factor

R_v = resistivity of electrolyte in the matrix, ohm-cm

R_o = resistivity of bulk electrolyte, ohm-cm

The equation relating the voltage drop caused by internal cell resistance is

$$E_{IR} = (R_v)(l)(i)$$

Where

E_{IR} = internal resistance voltage, volt

l = compressed matrix thickness, cm

i = cell current density, A/cm^2

For 55% Cs_2CO_3 charge concentration

E_{IR} = 0.037 volt

i = 0.0215 A/cm^2 (20 ASF)

R_o = 4.65 ohm-cm (at 66.5 F)

l = 0.0635 cm (0.025 in)

Therefore

$R_v = E_{IR}/(l)(i)$

$R_v = 0.037/(0.0635)(0.0215)$

R_v = 27.1 ohm-cm

$f = 27.1/4.65$

$f = 5.8$

For 61.5% Cs_2CO_3 charge concentration

$E_{IR} = 0.040$ volt

$i = 0.0215$ A/cm^2

$R_o = 4.69$ ohm-cm

$l = 0.0635$ cm

Therefore

$R_v = 0.040/(0.0635)(0.0215)$

$R_v = 29.3$

$f = 29.3/4.69$

$f = 6.2$

APPENDIX B AIR CAVITY MASS TRANSFER COEFFICIENT DERIVATION

The air cavity convective mass transfer coefficient, k_c, for the EDC can be estimated as a function of the Reynold's number and the Schmidt number. The equation for this functional relationship is

$$k_c = \left(\frac{D_{AB}}{L}\right) a\ Re^b Sc^c$$

Where

a, b and c = constants

D_{AB} = diffusion coefficient of CO_2 in air

L = diffusion length

Re = Reynold's number

Sc = Schmidt number

The following assumptions can be made:

1. Over the typical EDC operating temperature range (60-80F), the physical properties of air and CO_2 and the diffusion coefficient are constant.
2. The Schmidt number is approximately 1.0 (<5% error).
3. The Reynolds number is a function of the bulk air flow rate only.

Using these assumptions the equation for k_c reduces to

$$k_c = A\ V^b \qquad (1)$$

Where

A, b = constants

V = volumetric air flow rate

The value for k_c can be found experimentally by measuring the CO_2 removal efficiency and, hence, removal rate as a function of air flow rate for a low inlet pCO_2 level ($\leq$2.0 mm Hg where air cavity transfer is rate-limiting).

As previously shown, the equation for CO_2 removal is

$$N_{CO_2} = (k_c)(A)(M_{CO_2})(pCO_2 - pCO_2{}^o)/RT$$

Solving for k_c yields

$$k_c = N_{CO_2}\ RT/AM_{CO_2}\ (pCO_2 - pCO_2^{o}) \qquad (2)$$

In the air cavity mass transfer limiting region, pCO_2^{o} is assumed to be zero. The value of k_c can then be calculated by experimentally measuring N_{CO_2} for a given inlet pCO_2 and air flow rate. The values for k_c at each air flow rate tested (for a given inlet pCO_2) were least squares fit to equation (1) to give the value for A and b.

APPENDIX C COMPUTER PROGRAM DOCUMENTATION

```
CHI/OS  16 OCT 73:        RUN 2       LIFE SYSTEMS  (138900,0)                              21:40:22           DATE: 16 OCT 73


AB FOR
FORTRAN V - SEPTEMBER 20, 1973                                          TUESDAY, OCTOBER 16, 1973 AT 21:40:24
HIGHEST S.E. ADDRESS:     03110




000101               REALN,I
000103               COMMON A,B,C,D,EE,F,G,CPA,DHC,N,T2,T5,T6,HC,ETA,S(5,7)
000104               DATA S/1.75187,-.511449,.0775073,-.00592584,.000179862,
000104              &1.42306,-.271935,.0210187,-.00034839,-1.8475E-5,
000104              &1.08190,-.110821,-.0081408,.00196359,-8.5832E-5,
000104              &.90258,-.105068,.0025161,.00028694,-1.3673E-5,
000104              &.71551,-.072213,.0024297,9.08E-6,-3.48E-7,
000104              &.61612,-.055237,.0003803,.00028605,-1.5623E-5,
000104              &.52087,-.035109,-.0014939,.00035115,-1.4808E-5/
000104              &A,B,C,D,EE,F,G,CPA,CPH/3.2437814,.00586826,1.1702379E-8,
000104              &.0021878462,5.219603,273.16,2.3025851,1.0765,1.0666/
000117               IIN = 5
000120               IOUT = 6
000120         C     WHEN NFLAG=1 AND CERTAIN PARAMETERS ARE OUT OF RANGE,
000120         C     ONLY THE ASSOCIATED MESSAGES AND THE INPUT ARE PRINTED.
000120         C     WHEN NFLAG=0 A COMPLETE PRINTING IS DONE.
000121         1     READ(IIN,7001,END=9999) PC1,PO1PSA,P1PSA,T1,DP1,V1,
000121              &V3SL,T3,DP3,P3PSG,N,I,DELT1,T5,NFLAG
000142         7001  FORMAT(6F10.2/4F10.2/4F10.2,I10)
000143               WRITE(IOUT,230)
000145         230   FORMAT('1**********INPUT DATA**********')
000146               WRITE(IOUT,100)PC1,PO1PSA,P1PSA,T1,DP1,V1
000156         100   FORMAT('0CARD 1, PROCESS AIR IN:'/'       PC1    PO1PSA',
000156              &'      P1PSA          T1          DP1          V1'/6F10.2)
000157               WRITE(IOUT,102)V3SL,T3,DP3,P3PSG
000165         102   FORMAT('0CARD 2: H2 IN:'/'       V3SL          T3         DP3',
000165              &'      P3PSG'/ 4F10.3)
000166               WRITE(IOUT,104)N,I,DELT1,T5,NFLAG
000175         104   FORMAT('0CARD 3: MODULE:'/'          N          I      DELT1',
000175              &'          T5       NFLAG'/F10.0,3F10.2,I10)
000176               WRITE(IOUT,220)
000200         220   FORMAT('0***********RESULTS***********')
000201               NERROR=0
000201         C
000201         C     INLET PROCESS AIR CONVERSIONS:
000201         C
000202               P1=P1PSA*51.7007
000203               PO1=PO1PSA*51.7007
000204               PW1=PHTO(DP1)
000205               PN1=P1-PO1-PW1-PC1
000206               VW1=PW1/P1*V1
```

continued-

FIGURE C-1 SOURCE PROGRAM LISTING

Figure C-1 continued-

```
000207                V01=P01/P1*V1
000210                FW1=VW1*18.01*60./386.7
000211                FC1=V1*PC1/P1*44.01*60./386.7
000212                VC1=V1*PC1/P1
000213                RH1=PW1/PHTO(T1)*100.
000213          C
000213          C     INLET H2 CONVERSIONS:
000213          C
000214                V3=V3SL/28.32
000215                PW3=PHTO(DP3)
000216                P3=(P3PSG+14.7)*51.7007
000217                PH3=P3-PW3
000220                VW3=PW3/P3*V3
000221                VH3=V3-VW3
000222                FH3=VH3*60.*2.016/386.7
000222          C
000222          C     MODULE PARAMETER CALCULATIONS:
000222          C
000223                T2=DP1+DELT1
000224                E=.729-.22*ALOG(I)+.008*I+.005*(T2-78.)
000225                ESTACK=N*E
000226                CURDEN=I/.244
000227                POWER=ESTACK*I
000230                HEATLD=N*I*(1.25-E)*3.419
000231                OCON=6.5803E-4*N*I
000232                HCON=OCON*2.016/16.
000233                WPROD = OCON + HCON
000234                TI=TICOR(PC1,V1/N,CURDEN)
000235                TE=TI/.0275
000236                CTRANS=TI*OCON
000237                IF(FH3.GE.1.3*HCON)GO TO 1213
000241                V3MSL=1.3*HCON*V3*386.7*28.32/(VH3*2.016*60.)
000242                WRITE(IOUT,213)V3MSL
000245          213   FORMAT('0INSUFFICIENT HYDROGEN.  ',F10.2,' SLPM IS REQUIRED.')
000246                NERROR=1
000246          C
000246          C     COOLING AIR AND HEAT BALANCE CALCULATIONS:
000246          C     (HC, ETA AND T6 ARE CALCULATED IN FUNCTION ERT.)
000246          C
000247          1213  DHA=V1*CPA*(T2-T1)
000250                DHH=V3*CPH*(T2-T3)
000251                DHC=HEATLD-DHA-DHH
000252                IF(DHC.GE.0.)GO TO 898
000254                WRITE(IOUT,789)DHC
000257          789   FORMAT('0DHC =',1PG10.3,' BTU/HR.'/' INSUFFICIENT HEAT ',
000257               &'IS GENERATED TO MAINTAIN MODULE TEMPERATURE.')
000260          876   V5=0.
000261                HC=0.
000262                T6=0.
000263                ETA=0.
000264                NERROR=1
000265                GO TO 1430
000266          896   CONTINUE
000267                IF(T2-T5.GE..376*DHC/N)GO TO 765
```

Figure C-1 continued-

```
000271          WRITE(IOUT,987)
000273   987    FORMAT('0INSUFFICIENTLY LOW COOLING AIR TEMPERATURE.')
000274          GO TO 876
000275   765    CONTINUE
000276          VA=1.01*DHC/(CPA*N*(T2-T5))
000277          VB=2.*VA
000300          V5=N*ROOT(VA,VB,ERT,0.,.005,.001,10)
000301   1430   CONTINUE
000301   C      TRIAL VALUE OF DP4:
000302          DP4=T2-11.
000303          DO 937 NNNN=1,2
000303   C
000303   C      OUTLET H2 CALCULATIONS:
000303   C
000306          PW4=PHTO(DP4)
000307          FH4=FH3-HCON
000310          FC4=CTRANS
000311          VC4=FC4*386.7/44.01/60.
000312          VH4=VH3-HCON*386.7/60./2.016
000313          P4=P3
000314          VW4=PW4/(P4-PW4)*(VC4+VH4)
000315          FW4=VW4*60.*18.01/386.7
000316          V4=VH4+VW4+VC4
000317          CHWRTO=FC4/FH4
000320          HCVRTO=VH4/VC4
000321          VH4SL=VH4*28.32
000322          V4SL=V4*28.32
000323          VC4SL=VC4*28.32
000324          F4=FC4+FW4+FH4
000324   C
000324   C      OUTLET PROCESS AIR CALCULATIONS:
000324   C
000325          P2=P1
000326          FC2=FC1-CTRANS
000327          VC2=FC2*386.7/60./44.01
000330          VO2=VO1-OCON*386.7/32./60.
000331          VN2=PN1/P1*V1
000332          VW2=VW1+VW3+WPROD*386.7/60./18.01  - VW4
000333          V2=VO2+VN2+VW2+VC2
000334          PW2=P2*VW2/V2
000335          PC2=P2*VC2/V2
000336          DP2=DEWT(PW2)
000337          RH2=PW2/PHTO(T2)*100.
000340          FW2=VW2*18.01*60./386.7
000341          DP4=(DP1+DP2)*.5
000342   937    CONTINUE
000344          DELT1P=22.-T1+DP2
000345          T2P=DP1+DELT1P
000345   C
000345   C      MOISTURE BALANCE CHECKS:
000345   C
000346          IF(ABS(T1-DP1-11.25).LE.1.75
000346         &.AND. ABS(T2-DP2-11.25).LE.1.75)GO TO 30
000350          IF(T1-DP1.LT.4.)GO TO 1210
```

Figure C-1 continued

```
000552              IF(T1-DP1.GT.14.)GO TO 1210
000554              IF(T2-DP2.LT.7.)GO TO 1211
000556              IF(T2-DP2.GT.19.)GO TO 1211
000560              DPTDAV = .5*(T1-DP1+T2-DP2)
000561              IF(ABS(DPTDAV-11.).LE.1.5
000561             &.AND. (T2-DP2 .GE. 13. .OR. DPTDAV .GE. 15.))GO TO 30
000563              WRITE(IOUT,654)
000565      654     FORMAT('0AVERAGE PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.')
000566      28      WRITE(IOUT,543)
000570      543     FORMAT('0ELECTROLYTE MOISTURE BALANCE IS NOT MAINTAINED.')
000571      29      NERROR=1
000572      30      CONTINUE
000573              IF(NERROR*NFLAG.NE.0)GO TO 1
000573      C
000573      C       MAJOR OUTPUT SATEMENTS
000573      C
000575              WRITE(IOUT,106)T2,E,ESTACK,CURDEN,POWER,HEATLD,OCON,HCON,
000575             &WPROD, TI, TE, CTRANS
000413      106     FORMAT('0MODULE:'/8X,'T2',9X,'E',4X,'ESTACK',4X,'CURDEN',
000413             &5X,'POWER',4X,'HEATLD'/6F10.3//6X,'OCON',6X,'HCON',5X,'WPROD',
000413             &8X,'TI',8X,'TE',4X,'CTRANS'/3F10.5,3F10.4)
000414              WRITE(IOUT,101)PO1,P1,PW1,PN1,FW1,FC1,RH1,VO1,VW1
000427      101     FORMAT('0PROCESS AIR IN: '/'          PO1          P1          PW1',
000427             &7X,'PN1',7X,'FW1',7X,'FC1'/6F10.3//7X,'RH1',7X,'VO1',7X,'VW1'/
000427             &3F10.3)
000430              WRITE(IOUT,111)P2,PC2,PW2,V2,VC2,VW2,VN2,VO2,FC2,FW2,
000430             &DP2,RH2
000446      111     FORMAT('0PROCESS AIR OUT:'/'          P2        PC2         PW2',
000446             &8X,'V2',7X,'VC2',7X,'VW2'/4F10.2,2F10.4//7X,'VN2',7X,'VO2',
000446             &7X,'FC2',7X,'FW2',7X,'DP2',7X,'RH2'/6F10.3)
000447              WRITE(IOUT,103)V3,PW3,P3,PH3,VW3,VH3,FH3
000460      103     FORMAT('0H2 IN:'/'          V3        PW3         P3          PH3',
000460             &'       VW3        VH3        FH3'/F10.4,3F10.2,F10.6,F10.4,F10.6)
000461              WRITE(IOUT,110)DP4,PW4,FC4,VH4,VC4,P4,VW4,FW4,V4,V4SL,
000461             &VH4SL,VC4SL,FH4,F4,CHWRTO,HCVRTO
000503      110     FORMAT('0ANODE GAS OUT:'/'          DP4         PW4         FC4',
000503             &7X,'VH4',7X,'VC4',8X,'P4'/3F10.3,2F10.6,F10.2//7X,'VW4',7X,'FW4',
000503             &8X,'V4',6X,'V4SL',5X,'VH4SL',5X,'VC4SL'/2F10.6,4F10.4//
000503             &7X,'FH4',8X,'F4',4X,'CHWRTO',4X,'HCVRTO'/F10.6,3F10.4)
000504              WRITE(IOUT,109)DHA,DHH,DHC
000511      109     FORMAT('0HEAT BALANCE:'/'          DHA         DHH          DHC'/
000511             &3F10.3)
000512              WRITE(IOUT,107)V5,T5,T6,HC,ETA
000521      107     FORMAT('0COOLING AIR:'/'           V5          T5',
000521             &'          T6          HC          ETA'/5F10.3)
000522              WRITE(IOUT,456)DELT1P,T2P,DP1,DELT1P
000530      456     FORMAT('0PREFERRED VALUE OF DELT1 IS',F6.2,
000530             &' UNDER THESE CONDITIONS'/' SO THAT',F6.2,
000530             &' = T2 = DP1 + DELT1 =',F6.2,' +',F6.2,'.')
000531              GOTO1
000532      1210    WRITE(IOUT,432)
000534      432     FORMAT('0INLET PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.')
000535              GO TO 28
000536      1211    WRITE(IOUT,321)
```

Figure C-1 continued-

```
000540    321   FORMAT('0OUTLET PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.')
000541          GO TO 28
000542    9999  STOP
000542    C
000542    C     WATER VAPOR PRESSURE (PHTO) IS A FUNCTION OF DEW POINT (TF)
000542    C
000543          FUNCTIONPHTO(TF)
000546          REAL N,I
000547          COMMON A,B,C,D,EE,F,G,CPA,DHC,N,T2,T5,T6,HC,ETA
000550          TC=5.*(TF-32.)/9.
000551          X=374.11-TC
000552          PHTO=EXP(G*(EE-(X/(TC+F))*(A+B*X+C*X**3)/(1.0+D*X)))
000553          RETURN
000553    C
000553    C     DEW POINT (DEWT) IS A FUNCTION OF WATER VAPOR PRESSURE (P).
000553    C
000554          FUNCTION DEWT(P)
000557          REAL N,I
000560          COMMON A,B,C,D,EE,F,G,CPA,DHC,N,T2,T5,T6,HC,ETA
000561          EXTERNAL ROOT,PHTO
000562          XX=ALOG(P)
000563          TA=-2.4+20.25*XX+1.522*XX**2
000564          TB=TA+.1
000565          DEWT=ROOT(TA,TB,PHTO,P,.005,.005,5)
000566          RETURN
000566    C
000566    C     TRANSFER INDEX (TICOR) IS A FUNCTION OF INLET PCO2 (P),
000566    C     AIRFLOW PER CELL (AF), AND CURRENT DENSITY (CD).
000567          FUNCTION TICOR(P,AF,CD)
000572          REAL N,I
000573          COMMON A,B,C,D,EE,F,G,CPA,DHC,N,T2,T5,T6,HC,ETA,S(5,7)
000574          PA=P*(AF/.44)**(.45-.0045*P*P)
000575          J=CD/5.-1.
000576          IF(J.LT.1)J=1
000600          TI1=PA*(S(1,J)+PA*(S(2,J)+PA*(S(3,J)+PA*(S(4,J)+PA*S(5,J)))))
000601          IF(J.LT.7)GO TO 8
000603          TICOR=TI1
000604          RETURN
000605    8     J=J+1
000606          TI2=PA*(S(1,J)+PA*(S(2,J)+PA*(S(3,J)+PA*(S(4,J)+PA*S(5,J)))))
000607          AII=J
000610          TERP=CD/5.-AII
000611          TICOR=TI2*TERP+TI1*(1.-TERP)
000612          RETURN
000612    C
000612    C     FUNCTION ROOT RETURNS THE NUMBER -ROOT- SUCH THAT
000612    C     YFCN(ROOT) = W +OR- YTOL, AND SUCH THAT THE LAST
000612    C     CHANGE IN -ROOT- IS LESS THAN XTOL. MAXIMUM NUMBER
000612    C     OF ITERATIONS = K.  A SECANT FOLLOWING METHOD IS
000612    C     USED STARTING WITH X-VALUES X1 AND X2.
000612    C
000613          FUNCTION ROOT(X1,X2,YFCN,W,XTOL,YTOL,K)
000616          EXTERNAL YFCN
000617          XA=X1
```

Figure C-1 continued-

```
000620                XB=X2
000621                FA=YFCN(XA)-W
000622                FB=YFCN(XB)-W
000623                DO 91 IROOT=1,K
000626                XN=(FA*XB-FB*XA)/(FA-FB)
000627                FN=YFCN(XN)-W
000630                IF(ABS(FN).LT.YTOL .AND.
000630               &ABS(XN-XB).LT.XTOL)GO TO 99
000632                IF(IROOT.GE.K)WRITE(IOUT,200)X1,X2,W,XTOL,YTOL,IROOT,
000632               &XA,XB,XN,FA,FB,FN
000651      200       FORMAT('0NONCONVERGENCE IN ROOT',1P3E12.4/2E12.4,I3/6F12.4)
000652                XA=XB
000653                XB=XN
000654                FA=FB
000655                FB=FN
000656      91        CONTINUE
000660      99        ROOT=XN
000661                RETURN
000661      C
000661      C         FUNCTION ERT CALCULATES COOLING AIR EXIT TEMPERATURE (T6)
000661      C         FROM THE ENTRANCE TEMPERATURE (T5), HEAT DUTY (DHC),
000661      C         AND COOLING AIR FLOW PER CELL (V).  FROM T2, T5, AND T6
000661      C         THE LOG MEAN MODULE-COOLING AIR TEMPERATURE DRIVING
000661      C         FORCE IS CALCULATED.  THE DRIVING FORCE REQUIRED TO
000661      C         TRANSPORT THE HEAT THROUGH THE FINS AND INTO THE
000661      C         COOLING AIR IS CALCULATED.  THE DISCREPANCY BETWEEN
000661      C         THE AVAILABLE AND REQUIRED DRIVING FORCES IS RETURNED
000661      C         THROUGH THE VARIABLE ERT.  FIN EFFICIENCY (ETA) AND
000661      C         CONVECTIVE HEAT TRANSFER COEFFICIENT (HC) ARE ALSO CALCULATED.
000661      C
000662                FUNCTION ERT(V)
000665                REAL N,I
000666                COMMON A,B,C,D,EE,F,G,CPA,DHC,N,T2,T5,T6,HC,ETA
000667                IF(V.LE.1.)HC=1.97*V**(.3333)
000671                IF(V.GT.1. .AND. V.LT.2.9883)HC=1.21+V*(.34+.42*V)
000673                IF(V.GE.2.9883 .AND. V.LE.4.)HC=2.*V
000675                IF(V.GT.4.)HC=2.639016*V**(.8)
000677                ETA=1.
000700                IF(V.GT..32194 .AND. V.LT.24.72)ETA=1.0644-.1135*SQRT(V)
000702                IF(V.GE.24.72)ETA=2.486/SQRT(V)
000704                T6=T5+DHC/(V*CPA*N)
000705                DTREQ=DHC*(.376+3.876/(HC*ETA))/N
000706                IF(T6.LT.T2)GO TO 86
000710                ERT=-DTREQ
000711                RETURN
000712      86        DTAVA=(T6-T5)/ALOG((T2-T5)/(T2-T6))
000713                ERT=DTAVA-DTREQ
000714                RETURN
000715                END

  1 DIAGNOSTIC.
                                                                          2.5820 SECONDS.

END OF RUN:   DATE: 16 OCT 73   TIME: 21:52:57   CPU TIME:    2.59 SEC.   PAGES:    6     CARDS:   308 IN     0 OUT
```

TABLE C-1 NOMENCLATURE AND UNITS

Composite Variable Names

First Prefix	P	(Partial) Pressure, mm Hg
	V	Volume Flow Rate, Scfm 70F, 760 mm Hg
	F	Mass Flow Rate, Lb/Hr
	DP	Dew Point, F
	T	Temperature, F
	RH	Relative Humidity, %
Second Prefix	C	Carbon Dioxide (CO_2)
	O	Oxygen (O_2)
	N	Nitrogen (N_2)
	H	Hydrogen (H_2)
	W	Water (H_2O)
	(None)	Total Stream
Stream Number	1	Process Air Inlet
	2	Process Air Outlet
	3	H_2 Inlet
	4	H_2 Outlet
	5	Cooling Air Inlet
	6	Cooling Air Outlet
Units Suffix	(None)	Units of First Prefix
	PSA	Psia
	PSG	Psig
	SL	Slpm

Additional Variable Names

A,B,C,D,EE,F,G	Constants in pH_2O Dew Point Equation
AII,J	Indices Determine S Constants
CD	Current Density
CHWRTO	CO_2/H_2 Weight Ratio, Lb CO_2/Lb H_2
CPA	Volumetric Specific Heat, Air, Btu/Hr-Scfm-F
CPH	Volumetric Specific Heat, H_2, Btu/Hr-Scfm-F
CTRANS	CO_2 Transferred, Lb/Hr
CURDEN	Current Density, Amp/Ft^2
DELT1	Control Variable = T2-DP1, F
DHA	Enthalpy Gain of Inlet Process Air, Btu/Hr
DHC	Enthalpy Gain of Cooling Air, Btu/Hr
DHH	Enthalpy Gain of Inlet H_2, Btu/Hr
DPTDAV	Process Air Dew Point Depression, Average, F
DTAVA	Log Mean Available Temperature Drop, F
DTREQ	Required Module - Cooling Air Temperature Drop, F
E	Cell Voltage, Volt
ERT	Difference between DTREQ and DTAVA
ESTACK	Stack Voltage, Volt

continued -

Table C-1 - continued

ETA	Cooling Fin Efficiency, Dimensionless, 0-1
FA,FB,FN	Corresponding Dependent Values
HC	Cooling Fin Heat Transfer Coefficient, Btu/Hr-Ft^2-F
HCON	H_2 Consumption, Lb/Hr
HCVRTO	H_2/CO_2 Volume Ratio, Scfm H_2/Scfm CO_2
HEATLD	Net Heat Produced, Btu/Hr
I	Current, Amp
N	Number of Cells
NERROR	Check Violation Indicator 0 No Violation 1 Violation
NFLAG	Program Option Integer = 0 or 1
OCON	O_2 Consumption, Lb/Hr
P	Inlet pCO_2
PA	Inlet pCO_2 Corrected for Effect of Air Flow
POWER	Electrical Power Produced, Watt
S	Array containing Coefficients of PA in TI Correlation
TA,TB	Trial Values of Dew Point, F
TC,TF	Dew Point, C, F, respectively
TE	Current Efficiency, %
TERP	Current Density Interpolation Variable
TI	Transfer Index, Lb CO_2/Lb O_2
T2P	Preferred Value of T2
T11	TI at one of the seven current densities just below the desired current density
T12	TI at one of the seven current densities just above the desired current density
VA,VB	Trial Values for V5
WPROD	Water Production, Lb/Hr
X1,X2,XA,XB,XN	Trial Values of Independent Variable in Convergence

NOTE: Additional variable description is present in the comments of the source program listing.

APPENDIX D COMPUTER PROGRAM SAMPLE OUTPUTS

```
**********INPUT DATA**********
CARD 1, PROCESS AIR IN:
      PC1    PO1PSA     P1PSA        T1       DP1        V1
     3.00      3.10     14.70     57.00     46.00     40.00
CARD 2: H2 IN:
     V3SL        T3       DP3     P3PSG
   10.500    70.000    46.000     5.000
CARD 3: MODULE:
        N         I     DELT1        T5     NFLAG
      90.      4.88     20.00     57.00         1

***********RESULTS***********

MODULE:
       T2         E    ESTACK    CURDEN     POWER    HEATLD
   66.000     0.359    32.338    20.000   157.808  1337.485

     OCON      HCON     WPROD        TI        TE    CTRANS
  0.28901   0.03641   0.32542    2.1713   78.9571    0.6275

PROCESS AIR IN:
      PO1        P1       PW1       PN1       FW1       FC1
  160.272   760.000     7.929   588.799     1.166     1.078

      RH1       VO1       VW1
   66.609     8.435     0.417

PROCESS AIR OUT:
       P2       PC2       PW2        V2       VC2       VW2
   760.00      1.26     10.15     39.97    0.0660    0.5336

      VN2       VO2       FC2       FW2       DP2       RH2
   30.989     8.377     0.451     1.491    52.614    62.008

H2 IN:
       V3       PW3        P3       PH3       VW3       VH3       FH3
   0.3708     7.929     1019.     1011. 2.886E-03    0.3679    0.1151

ANODE GAS OUT:
      DP4       PW4       FC4       VH4       VC4        P4
   49.307     8.971     0.628  0.251461  0.091897   1018.50

      VW4       FW4        V4      V4SL     VH4SL     VC4SL
 0.003051  0.008527    0.3464    9.8103    7.1214    2.6025

      FH4        F4    CHWRTO    HCVRTO
 0.078657    0.7147    7.9780    2.7363

HEAT BALANCE:
      DHA       DHH       DHC
  387.540    -1.582   951.527
```

```
COOLING AIR:
       V5          T5          T6          HC         ETA
   626.416      57.000      58.411      12.461       0.765

PREFERRED VALUE OF DELT1 IS 17.61 UNDER THESE CONDITIONS
SO THAT 63.61 = T2 = DP1 + DELT1 = 46.00 + 17.61.



**********INPUT DATA**********
CARD 1, PROCESS AIR IN:
        PC1      PO1PSA       P1PSA          T1         DP1          V1
       3.00        3.10       14.70       51.00       46.00        0.80
CARD 2: H2 IN:
       V3SL          T3         DP3       P3PSG
      0.300      70.000      46.000       0.000
CARD 3: MODULE:
          N           I       DELT1          T5       NFLAG
         1.        2.44       20.00       51.00           1

**********RESULTS************

DHC =      -6.55 BTU/HR.
INSUFFICIENT HEAT IS  GENERATED TO MAINTAIN MODULE TEMPERATURE.


**********INPUT DATA**********
CARD 1, PROCESS AIR IN:
        PC1      PO1PSA       P1PSA          T1         DP1          V1
       2.80        3.10       14.70       68.00       57.00        0.44
CARD 2: H2 IN:
       V3SL          T3         DP3       P3PSG
      0.300      70.000      46.000       0.000
CARD 3: MODULE:
          N           I       DELT1          T5       NFLAG
         1.        4.88       20.00       68.00           0

**********RESULTS************

AVERAGE PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.

ELECTROLYTE MOISTURE BALANCE IS NOT MAINTAINED.

MODULE:
         T2           E      ESTACK      CURDEN       POWER      HEATLD
     77.000       0.414       0.414      20.000       2.022      13.943

       OCON        HCON       WPROD          TI          TE      CTRANS
    0.00321     0.00040     0.00362      2.0877     75.9163      0.0067

PROCESS AIR IN:
        PO1          P1         PW1         PN1         FW1         FC1
    160.272     760.000      11.903     585.025       0.019       0.011

        RH1         VO1         VW1
     67.888       0.093       0.007
```

```
PROCESS AIR OUT:
       P2       PC2       PW2        V2       VC2       VW2
   760.00      1.11     14.04      0.44    0.0006    0.0081

      VN2       VO2       FC2       FW2       DP2       RH2
    0.339     0.092     0.004     0.023    61.623    59.103

H2 IN:
       V3       PW3        P3       PH3       VW3       VH3       FH3
1.059E-02     7.929     760.0     752.1 1.105E-04 1.048E-02 3.279E-03

ANODE GAS OUT:
      DP4       PW4       FC4       VH4       VC4        P4
   59.311    12.894     0.007  0.009189  0.000982    760.00

      VW4       FW4        V4      V4SL     VH4SL     VC4SL
 0.000176  0.000491    0.0103    0.2930    0.2602    0.0278

      FH4        F4    CHWRTO    HCVRTO
 0.002874    0.0101    2.3323    9.3599

HEAT BALANCE:
      DHA       DHH       DHC
    4.263     0.079     9.601

COOLING AIR:
       V5        T5        T6        HC       ETA
    5.449    68.000    69.637    10.244     0.799

PREFERRED VALUE OF DELT1 IS 15.62 UNDER THESE CONDITIONS
SO THAT 72.62 = T2 = DP1 + DELT1 = 57.00 + 15.62.

***********INPUT DATA***********
CARD 1, PROCESS AIR IN:
      PC1    PO1PSA     P1PSA        T1       DP1        V1
     1.50      3.10     14.70     51.00     46.00     40.00
CARD 2: H2 IN:
     V3SL        T3       DP3     P3PSG
    1.000    70.000    46.000     0.000
CARD 3: MODULE:
        N         I     DELT1        T5     NFLAG
      90.      4.88     20.00     40.00         0

************RESULTS************

INSUFFICIENT HYDROGEN.        4.33 SLPM IS REQUIRED.

AVERAGE PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.

ELECTROLYTE MOISTURE BALANCE IS NOT MAINTAINED.
```

```
MODULE:
       T2         E    ESTACK    CURDEN     POWER    HEATLD
   66.000     0.359    32.338    20.000   157.808  1337.485

     OCON      HCON     WPROD        TI        TE    CTRANS
  0.28901   0.03641   0.32542    1.3601   49.4578    0.3931

PROCESS AIR IN:
      PO1        P1       PW1       PN1       FW1       FC1
  160.272   760.000     7.929   590.299     1.166     0.539

      RH1       VO1       VW1
   82.933     8.435     0.417

PROCESS AIR OUT:
       P2       PC2       PW2        V2       VC2       VW2
   760.00      0.41     10.15     40.00    0.0214    0.5344

      VN2       VO2       FC2       FW2       DP2       RH2
   31.068     8.377     0.146     1.493    52.632    62.049

H2 IN:
       V3       PW3        P3       PH3       VW3       VH3       FH3
3.531E-02     7.929     760.0     752.1 3.684E-04 3.494E-02 1.093E-02

ANODE GAS OUT:
      DP4       PW4       FC4       VH4       VC4        P4
   49.316     8.981     0.393  -.081473  0.057563    760.00

      VW4       FW4        V4      V4SL     VH4SL     VC4SL
 -.000286  -.000799    -.0242    -.6852   -2.3073    1.6302

      FH4        F4    CHWRTO    HCVRTO
 -.025485    0.3668  -15.4239   -1.4154

HEAT BALANCE:
      DHA       DHH       DHC
  645.900     -.151   691.736

COOLING AIR:
       V5        T5        T6        HC       ETA
   62.883    40.000    50.219     1.748     0.970

PREFERRED VALUE OF DELT1 IS 23.63 UNDER THESE CONDITIONS
SO THAT 69.63 = T2 = DP1 + DELT1 = 46.00 + 23.63.
```

```
**********INPUT DATA**********
CARD 1, PROCESS AIR IN:
      PC1     P01PSA      P1PSA         T1        DP1         V1
    10.00       3.10      14.70      51.00      46.00      40.00
CARD 2: H2 IN:
     V3SL         T3        DP3      P3PSG
   20.000     70.000     46.000      0.000
CARD 3: MODULE:
        N          I      DELT1         T5      NFLAG
      90.       4.88      20.00      90.00          0

***********RESULTS************

INSUFFICIENTLY LOW COOLING AIR TEMPERATURE.

AVERAGE PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.

ELECTROLYTE MOISTURE BALANCE IS NOT MAINTAINED.

MODULE:
       T2          E     ESTACK     CURDEN      POWER     HEATLD
   66.000      0.359     32.338     20.000    157.808   1337.485

     OCON       HCON      WPROD         TI         TE     CTRANS
  0.28901    0.03641    0.32542     2.6488    96.3200     0.7655

PROCESS AIR IN:
      P01         P1        PW1        PN1        FW1        FC1
  160.272    760.000      7.929    581.799      1.166      3.594

      RH1        V01        VW1
   82.933      8.435      0.417

PROCESS AIR OUT:
       P2        PC2        PW2         V2        VC2        VW2
   760.00       7.88      10.14      39.95     0.4142     0.5328

      VN2        V02        FC2        FW2        DP2        RH2
   30.621      8.377      2.828      1.489     52.590     61.953

H2 IN:
       V3        PW3         P3        PH3        VW3        VH3        FH3
   0.7062      7.929      760.0      752.1  7.368E-03     0.6988     0.2186

ANODE GAS OUT:
      DP4        PW4        FC4        VH4        VC4         P4
   49.295      8.957      0.766   0.582432   0.112106     760.00

      VW4        FW4         V4       V4SL      VH4SL      VC4SL
 0.008283   0.023146     0.7028    19.9039    16.4945     3.1748

      FH4         F4     CHWRTO     HCVRTO
 0.182185     0.9709     4.2019     5.1954
```

```
HEAT BALANCE:
      DHA         DHH         DHC
  645.900      -3.013     694.598

COOLING AIR:
       V5          T5          T6          HC         ETA
    0.000      90.000       0.000       0.000       0.000

PREFERRED VALUE OF DELT1 IS 23.59 UNDER THESE CONDITIONS
SO THAT 69.59 = T2 = DP1 + DELT1 = 46.00 + 23.59.

**********INPUT DATA**********
CARD 1, PROCESS AIR IN:
      PC1      PO1PSA       P1PSA          T1         DP1          V1
     3.00        3.10       14.70       51.00       46.00       20.00
CARD 2: H2 IN:
     V3SL          T3         DP3       P3PSG
    5.000      70.000      46.000       0.000
CARD 3: MODULE:
        N           I       DELT1          T5       NFLAG
      45.        9.76       25.00       51.00           0

***********RESULTS***********

AVERAGE PROCESS AIR DEW POINT DEPRESSION OUT OF RANGE.

ELECTROLYTE MOISTURE BALANCE IS NOT MAINTAINED.

MODULE:
       T2           E      ESTACK      CURDEN       POWER      HEATLD
   71.000       0.271      12.189      40.000     118.960    1470.307

     OCON        HCON       WPROD          TI          TE      CTRANS
  0.28901     0.03641     0.32542      1.2349     44.9043      0.3569

PROCESS AIR IN:
      PO1          P1         PW1         PN1         FW1         FC1
  160.272     760.000       7.929     588.799       0.583       0.539

      RH1         VO1         VW1
   82.933       4.218       0.209

PROCESS AIR OUT:
       P2         PC2         PW2          V2         VC2         VW2
   760.00        1.01       12.36       20.01      0.0267      0.3255

      VN2         VO2         FC2         FW2         DP2         RH2
   15.495       4.159       0.182       0.910      58.057      63.649

H2 IN:
       V3         PW3          P3         PH3         VW3         VH3         FH3
   0.1766       7.929       760.0       752.1   1.842E-03      0.1747   5.465E-02
```

```
ANODE GAS OUT:
      DP4       PW4       FC4       VH4       VC4        P4
   52.028     9.923     0.357  0.058296  0.052264    760.00

      VW4       FW4        V4      V4SL     VH4SL     VC4SL
 0.001463  0.004087    0.1120    3.1725    1.6509    1.4801

      FH4        F4    CHWRTO    HCVRTO
 0.018235    0.3792   19.5713    1.1154

HEAT BALANCE:
      DHA       DHH       DHC
  430.600     0.188  1039.519

COOLING AIR:
       V5        T5        T6        HC       ETA
  299.394    51.000    54.225    12.019     0.772

PREFERRED VALUE OF DELT1 IS 29.06 UNDER THESE CONDITIONS
SO THAT 75.06 = T2 = DP1 + DELT1 = 46.00 + 29.06.
```