COMPUTER SIMULATION OF THE NASA WATER VAPOR ELECTROLYSIS REACTOR

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ABSTRACT

A digital computer simulation of the water vapor electrolysis reactor, an oxygen regenerator to be used in extended-mission manned spacecraft, was developed as a design tool and as a means for predicting response to unusual operating conditions. Finite increment analysis was applied to the mass, heat, and momentum transfer processes of the unit, yielding systems of non-linear algebraic equations defining the reactor. Pseudo-linear Seidel and non linear Rudd iteration schemes provided solutions to the descriptive equations. Compared with experimental data, the model predicted measurable quantities within one percent and, additionally, yielded information never before measured.

I. INTRODUCTION

The water vapor electrolysis (WVE) reactor is a spacecraft waste reclamation system for extended-mission manned spacecraft, Skylab or the flight to Mars for example. The WVE reactor's raw material is water, its product oxygen. Water is a metabolic waste produced in excess. Part of the excess is exhaled and perspired water vapor, containing more than enough oxygen to satisfy a person's nominal two-pound daily requirement. Electrolysis can free that oxygen, and that is basically the function of the WVE process, providing oxygen for breathing as well as necessary spacecraft dehumidification.

The WVE process was developed experimentally by empirical means. It was considered that a theoretically sound approach would provide more useful information concerning the WVE reactor, hence a better design. The goal of the work, then, was a rigorous design tool, a mathematical analog of an operating WVE reactor capable of generating any information quickly and accurately, from any given set of independent design variables.

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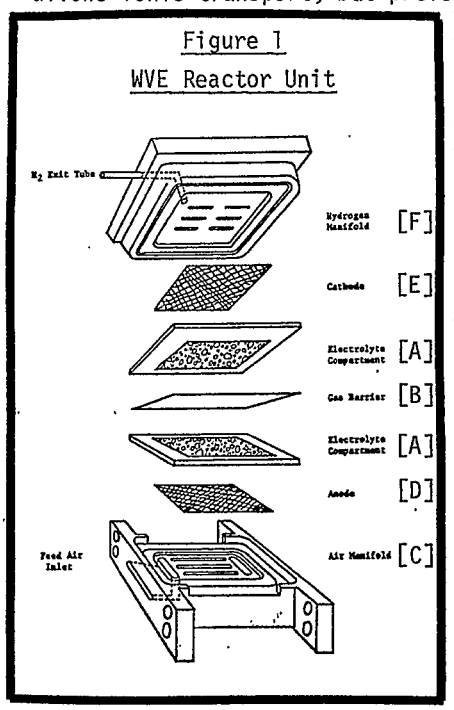
II. WVE REACTOR ANALYSIS

A unit of a WVE reactor is shown in Figure 1. The unit's electrolysis cell has two thin rectangles of electrolyte [A] separated by a microporous PVC membrane [B]. The electrolyte is concentrated sulfuric acid, immobilized for operation under acceleration and free fall by gelling with silica. The membrane allows ionic transport, but prevents passage of product gases. Water vapor, from the air flowing in the feed/product channel [C], is absorbed by the sulfuric acid thru the screen electrode [D]. Oxygen is evolved at that electrode and is swept away, along with the heat of anodic reaction, in the air stream. Hydrogen, the by-product of the water electrolysis reaction, evolves at the cathode [E] and exits the unit in a separate outlet stream [F].

Figure 1
WVE Reactor Unit



Analysis of the processes of the electrolysis cell yielded a system of 12 equations in 17 unknowns, all non-linear, 4 non-analytical. The independent variables were cell voltage, electrode type and spacing, and masses of silica and H_2SO_4 in the aqueous electrolyte gell. The primary dependent variable, oxygen production rate (cell current) further depended upon heat and mass transfer between the cell and the air stream.

Since air lost humidity and gained heat as it traveled across the anode through the channel, driving forces for heat and mass transfer were variable along the length of the cell, causing all the dependent variables of the electrolysis cell equations to be variable with position. Over a small increment of the cell length, however, properties could be approximated as constant, allowing the system of equations to be solved.

For the air channel, there is no analytical solution for the problem at hand, entrance region laminar flow of a compressible Newtonian fluid through a duct with variable heat and mass transfer at one wall. Finite increment analysis transformed the problem to the solution of a system of algebraic equations. The basis was an element (I,J) positioned (I) small increments from the channel inlet and (J) small increments from the cell anode. Equations were written describing the conservation of mass, momentum, and energy entering and leaving the element. Four non-linear conservation equations and the gas law described each element. Boundary conditions necessary for determinacy were the heat and mass transfer at each point (I) along the interface between the air channel and the cell anode. Independent variables were the inlet air's temperature, pressure, humidity, and velocity profile, and the air channel dimensions.

III. SOLUTION OF THE DESCRIPTIVE EQUATIONS

The solution of the equations describing the electrolysis cell at (I) increments from the channel inlet required an iterative numerical algorithm. The partially non-analytic nature of the system of equations made the usual methods of solution of non-linear equation systems cumbersome at best. The 'Design Variable Selection Algorithm' (4), developed as a chemical process design aid, yielded a simple stepwise form and order of solution for the system. Operations on the 'Rudd Array' for the system showed that a minimum of two variables required being 'guessed' at the start of each iteration. Heat and mass transfer at the anode were selected, being the interface boundary conditions. The algorithm gives no clue as to the values for guesses at the start of each iteration which would lead to convergence. A trial and error procedure was employed, and the simplest scheme giving non-oscillatory convergence was used.

For N elements (I,J) in row (I) of the air channel, there were 5N equations to be solved, plus the two boundary conditions. Assuming bulk flow dominance, the variables of row (I) could be solved for using only information known from row (I-1) and the boundary conditions. Since the inlet air's properties, row (I=0), were known, the rows (I) could be dealt with sequentially. The various popular algorithms for the solution of systems of non-linear equations applied to the algebraic equations, but none worked well. Another method was tried. While each of the equations for an element was non-linear, each of the five was linear in a unique variable. Treating the non-linear terms as 'transitory constant' coefficients of the linear terms allowed the methods of linear equation problem solving. Since the transitory constants needed numerical values for digital computer solution, the algorithm was iterative, a modification of the Seidel method. As the algorithm converged, the values of the transitory constants approached their true values.

The simulation of the WVE reactor proceeded from the air channel inlet to the exit in increments. Estimations of heat and mass transfer at the anode at an increment allowed solution of the air channel equations. The electrolysis cell equations then were used to calculate better estimations of heat and mass transfer at that point. The cycle was then repeated until the estimations converged. Then the next increment along the reactor length was acted upon in the same way, and so on until the end of the channel.

IV. RESULTS OF THE SIMULATION

The simulation was a theoretically rigorous analog of a WVE reactor unit, with all degrees of freedom intact. Assumptions made for computational simplicity either invalidated the model far outside its region of normal operation, or were shown valid by independent calculation. The FORTRAN IV routine executed in about 100 seconds using 23K of 360/67 core.

Of the dependent variables, only cell current and exit air properties had been measured experimentally, and at only four different sets of conditions (1,2,3,5). Using the same four independent variable vectors, simulation output deviated from measured values by an average of one percent, error ranging from zero to two percent.

Since any datum at any point in the WVE reactor was accessible via the simulation, more data was generated than had ever been measured. Of design interest were the variations of current density, cell temperature, and electrolyte concentration within the reactor, previously only postulated. In addition to the extra data the simulation was far superior to experiment in the time needed to measure the response to a change in the independent variable vector, 100 seconds versus two to ten days (1). In generating far more accurate data far more quickly than by experiment, the simulation proved its worth, and the goal of the work was met.

REFERENCES

1. Bloom, A M, Process Analysis and Efficiency Studies of the Water Vapor Electrolysis Cell, The Pennsylvania State University, The Graduate School, 1972.
2. Clifford, J E, 'Water Vapor Electrolysis With Phosphoric Acid Electrolyte," SAE Aeronautic and Space Engineering and Manufacturing Meeting, Los Angeles, Cal, 1967.
3. Connor, W J et. al., Final Report, NASA Contract No. NAS 2 2156, Lockheed Missiles and Space Co., 1969.
4. Lee, W et. al., AIChEJ, No. 6, 12, 1966.
5. Wydevan, T and E Smith, 'Water Vapor Electrolysis,' Aerospace Medicine, 1045, 1967.

BIOGRAPHY

ALLAN MAURICE BLOOM, Information Systems Department, The Pennsylvania State University, received his Ph D in 1972. He is currently involved in research into increasing programmer productivity via dictation of computer programs. He is a graduate of both the University of Pennsylvania and The Pennsylvania State University.