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ADVANCED ETC/LSS COMPUTERIZED ANALYTICAL MODELS - CO_2 CONCENTRATION
FINAL REPORT

VOLUME II Simulation Manual

MCDONNELL DOUGLAS ASTRONAUTICS COMPANY

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CORPORATION

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ADVANCED ETC/LSS COMPUTERIZED ANALYTICAL MODELS – CO_2 CONCENTRATION FINAL REPORT

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Simulation Manual

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FOREWORD

The study described in this report was prepared by the Biotechnology and Power Department of the Advance Systems and Technology Directorate, McDonnell Douglas Astronautics Company - Western Division, Huntington Beach, California. J. R. Jaax, Crew Systems Division, National Aeronautics and Space Administration, Manned Spacecraft Center (MSC) was the contract technical monitor. B. N. Taylor was the principal investigator for McDonnell Douglas. A. V. Loscutoff assisted in the preparation of the computer subroutines and simulation models. Volume I of this report is a summary of the work performed. Volume II contains detailed information concerning the preparation and usage of the analytical models.

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SUMMARY

Computer simulations have been prepared for the concepts of CO_2 concentration which have the potential for maintaining a CO_2 partial pressure of 3.0 mmHg, or less, in a spacecraft environment. The simulations were performed using the G-189A Generalized Environmental Control computer program. In preparing the simulations, new subroutines to model the principal functional components for each concept were prepared and integrated into the existing program. Sample problems are presented within this report which demonstrate the methods of simulation and performance characteristics of the individual concepts. Comparison runs for each concept can be made for parametric values of cabin pressure, crew size, cabin air dry and wet bulb temperatures, and mission duration.

The computer simulations have pointed out that, for many of the concepts, additional laboratory testing is required to determine better data for certain subsystems parameters or physical properties. Specific recommendations for each concept are contained in section 3.0 of this report.

The analytical models provide a means of determining subsystem performance for the concepts for a wide range of operating conditions. This should aid in an evaluation of the relative merits of each concept to satisfy various mission requirements.

1.0 INTRODUCTION

The maximum allowable CO_2 partial pressure for future manned space programs has been set at 3.0 mm Hg. This has required an evaluation of all CO_2 management concepts capable of meeting the 3.0 mm Hg or less constraint. Ten concepts which have potential for meeting this requirement are listed below:

- steam desorbed solid amines
- vacuum desorbed solid amines
- carbonation cell
- hydrogen depolarized cell
- solid electrolyte
- liquid absorption
- electrodialysis
- molten carbonate
- membrane diffusion
- mechanical freezout

The above-mentioned concepts are in various stages of development. The steam desorbed reins concept has been tested in the 90-day manned simulator run. Extensive development work has been performed on the hydrogen depolarized cell concept for use in the Space Station Prototype (SSP) EC/LS being developed for NASA Manned Spacecraft Center (MSC). The molten carbonate concept is an example of a concept for which many design problems must be solved before a viable design is evolved.

In order to assist in the evaluation of the relative merits of each concept, computer subroutines have been developed for simulating the performance characteristics of the concepts.

The subroutines have been integrated into the G-189A Generalized Environmental Control computer program. A brief description of this computer program is contained in Appendix A of this report. Using the program, each concept can thus be evaluated for a wide variety of operational design conditions. The following conditions have been specified as design parameters:

o	cabin total pressure	10 - 14.7 psia
o	crew size	2 - 12
o	dry bulb temperature	65 - 75°F
o	wet bulb temperature	46 - 57°F
o	O_2 partial pressure	3.1 to 3.5 psia
o	cabin diluent gas	nitrogen
o	gravity conditions	0 - 1.0g
o	CO_2 production rate	1.9 to 3.0 lb/man-day
o	mission time	0.5 to 10 years

A generalized rather than specific approach has been used in preparing the simulation of the concepts. A typical concept was modeled by breaking up the subsystem into a series of functional components. These functional components might be an absorbing or desorbing bed, several heat exchangers or dehumidifiers, control valves, fans, etc. Existing G189A subroutines are available for simulating many of the functional components. New subroutines were prepared when required. For those components which have a common function in more than one concept, a single routine was prepared which could be used in simulating both concepts. For example, the same routine is used for simulating the absorption phase of operation for both the steam desorbed and vacuum desorbed resin concepts.

The subroutines used, order in which they are solved, sources of flow to a component are specified as input data to the G189A program. Any arbitrary arrangement can be simulated. The program has a considerable amount of flexibility for reflecting subsystem design or operating changes.

The simulation of a CO_2 concentrator using the G189A may require incorporation of a considerable amount of additional coding to simulate interfaces between components. This results from the cyclical operation of many of the concepts. Time sequencing valves may change the direction of flow from one component to another. For instance, when absorbing a bed received its flow (air) from one source, but while desorbing the same bed receives its flow (steam) from another source. Thus coding may be necessary to interpolate tables specifying the cyclical operation of the bed, alter the order of component solution, and change the source of flow. This coding may be incorporated into G-189A subroutine GP0LY or into a special purpose subroutine to simulate the interface function.

Sample problems have been prepared to illustrate the simulation of each concept. Descriptions of the new subroutines prepared are given in the Appendix. Data input requirements and the analytical model used are included in the description.

The methods of simulation described and the new subroutines prepared will allow comparative evaluation of the performance of each concept. In particular, the capacity of a particular design for maintaining a 3.0 mm Hg CO_2 partial pressure may be evaluated. Parametric runs for specified conditions of cabin pressure and volume, crew size, or CO_2 production rate, cabin air dry and wet bulb temperatures, gravity, and mission duration may be made. Alternatively, each concept can be evaluated for assumed values of CO_2 flow rates to the subsystem and comparing the time averaged values for removal rates. The impact of interfaces with other subsystems such as oxygen regeneration or water recovery also can be determined. This should aid in selection of the optimum subsystem and suitable alternatives for a particular space mission.

2.1 STEAM DESORBED RESINS

2.1.1 Process Description

In this CO_2 concentration process, cabin air passes through a granular bed of solid amine particles such as amberlite IR-45 resin. Since amines are weak bases, carbon dioxide (an acid gas) undergoes a weak chemical reaction with the sorbent and is therefore removed from the cabin air.

As more and more carbon dioxide absorbs in the resin, a point will finally be reached when the CO_2 in the gas stream comes to equilibrium with the CO_2 absorbed in the resin. At this time, the resin will have picked up all the CO_2 it is capable of holding and must then be regenerated.

In the steam desorb resin concept, regeneration is accomplished by passing superheated steam through the bed. Trapped air in the void space between particles is first pushed out. After elution of the air, carbon dioxide is the main effluent. When the CO_2 is essentially depleted, steam-breakthrough occurs. Regeneration is then complete.

MSA Research Corporation, References 1.1 and 1.2, conducted fundamental studies on CO_2 sorbents for NASA Langley Research Center. An ion-exchange resin, amberlite IR-45, manufactured by the Rohm and Haas Company proved to be durable and suitable for practical CO_2 removal processes.

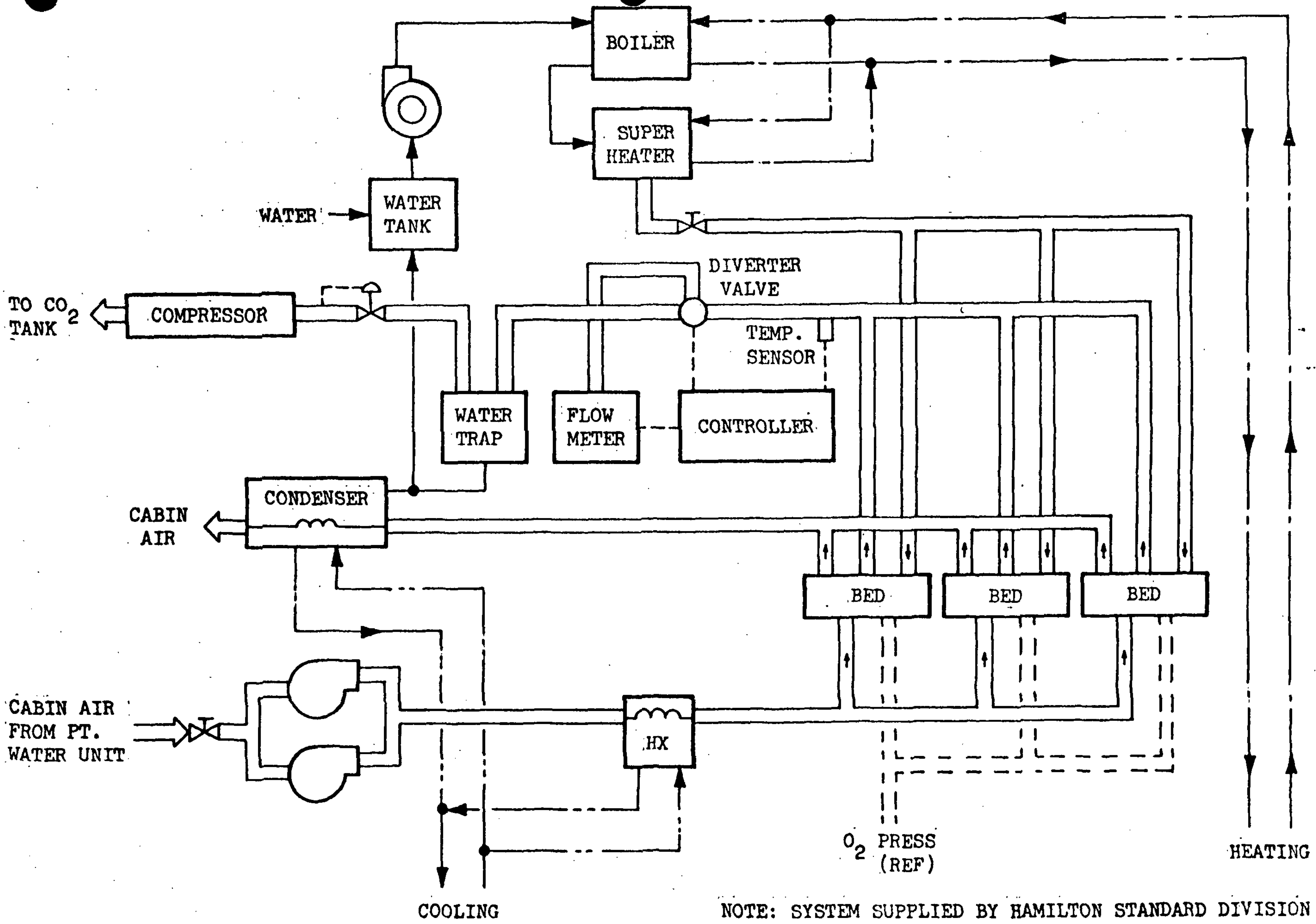
Hamilton Standard utilized surplus flight hardware from the MOL program to fabricate a solid-amine carbon dioxide concentrator. The performance of the unit was demonstrated in the 90-day manned test of MDAC, Reference 1.3.

2.1.2 Process Operational Details

CO_2 is removed from cabin air by means of cyclic absorption/desorption in suitable granular amine resins. The chemical nature of the bonding between CO_2 and these resins provides a CO_2 removal method which is feasible for cabin P_{CO_2} levels of 3 mm Hg or less. Dynamic CO_2 absorption and desorption processes, as well as equilibrium CO_2 bed loading conditions, are extremely sensitive to the amount of water present. For example, for IR-45 resin, increases in bed water content up to as high as 40% weight result in corresponding increased absorption efficiencies (Reference 1.1). However, water vapor contents higher than 25% have been shown to cause excessive pressure drop and flooding. With the bed cooler than approximately 140°F the absorption process takes place according to the following relationship:

$$R * NH_2 + CO_2 + H_2O \longrightarrow RNH_3^+ + HCO_3^-$$

For steam desorbed resins, desorption is accomplished by flowing superheated steam into the bed in the axial direction. The steam condenses on the resin, heats the resin and displaces the CO_2 and air. The process occurs in "chromatographic" fashion. That is, steam, CO_2, and air are found in individual zones which travel along the length of the bed. See Reference 1.1. The displaced CO_2 is reabsorbed immediately ahead of the steam zone and the air is displaced ahead of the CO_2-rich zone. This chromatographic feature of the absorption process facilitates separation of CO_2 from air and steam. Flows of the separate quantities of gas in each of the zones have associated physical properties which can be sensed and used in control schemes for diverting the CO_2-rich flow to the CO_2 accumulator and also for diverting the air and steam flows back to the cabin via a condensing heat exchanger. Two of these properties which have been used in the steam desorbed resin CO_2 concentrator for the LaRC/MDAC 90-day manned test are gas temperature and flow rate. See Figure 2.1-1. CO_2 has a higher mass flow rate out of the bed than air does due in part to its higher molecular weight and, therefore, higher density. The increase in



NOTE: SYSTEM SUPPLIED BY HAMILTON STANDARD DIVISION OF UNITED AIRCRAFT CORPORATION

FIGURE 2.1-1 NASA/MDAC 90-DAY MANNED TEST AMINE RESIN-CO_2 CONCENTRATOR SYSTEM mass flow rate which occurs as the air zone is depleted and the CO_2 zone elutes from the bed is sensed and a controller actuates a valve which diverts the CO_2 to the CO_2 accumulator. As the CO_2 zone is depleted, an increase in gas temperature at the bed exit plane occurs as steam commences to leave the bed. This temperature is sensed and the control valve is actuated to divert the flow back to the cabin return line. The effluent steam is condensed in the condensing heat exchanger in this line and the resulting condensate is returned to the water boiler. With steam desorbed resins the desorption phase of the process generally occurs at total gas pressures in the vicinity of cabin pressure. The pressure of the CO_2-rich gas leaving the bed is raised in a compressor to a pressure slightly in excess of CO_2 accumulator pressure. Since accumulator pressures are often in the order of 50 psia or less, the required compressor pressure ratio and associated power are considerably less than they are for CO_2 concentrator methods which utilize vacuum desorption.

Following desorption, the beds are hot and moist. Cabin atmosphere entering a bed during the absorption phase of the process is maintained at a suitable inlet temperature (65°F - 85°F) and the inlet humidity is maintained above a lower limit (∿ 35% RH). Initially this entering air is heated by the hot moist bed. Heat is removed from the air in evaporating moisture from the bed. When desirable operating conditions are achieved, the amount of water condensed and partially absorbed in the bed during the desorption phase is exactly balanced by that evaporated during the absorption phase and the water content in the bed during absorption remains high enough to enhance CO_2 absorption.

Figure 2.1-2 shows representative performance data for the steam desorbed resin CO_2 concentrator used in the LaRC/MDAC 90-day manned test. These data were recorded during "two-bed operation." That is, two of the three available absorption beds are operating and the adsorption and desorption cycles were of equal duration. The lower curve shows the mixed P_{CO_2} downstream of the two absorption beds. As shown, the effluent P_{CO_2} drops rapidly at the start of the absorption phase, reaches a minimum value, and then rises with a plateau characteristic observed partway through the P_{CO_2} rise. This plateau characteristic was also reported in Reference 1.1. Again, in Figure 2.1-2 it is seen that most of the absorption occurs early in the absorption phase. The latter portion of the absorption phase was mainly used in drying the bed prior to the next desorption phase.

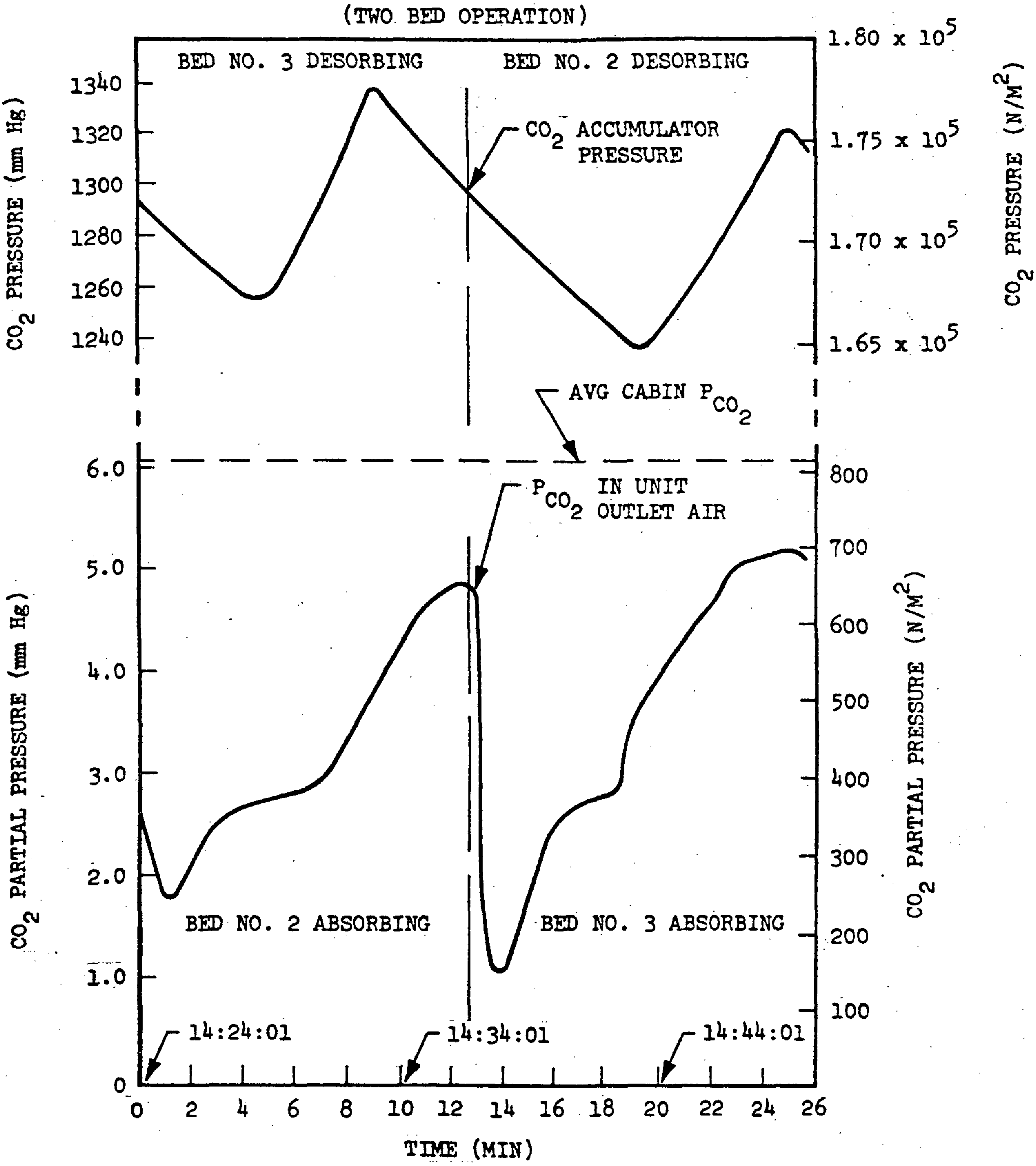


FIGURE 2.1-2 NASA/MDAC 90-DAY MANNED TEST
AMINE RESIN CO_2 CONCENTRATOR PERFORMANCE

The upper curve on Figure 2.1-2 shows the P_{CO_2} in the accumulator. The negative slope portions of the curve are due to CO_2 removal for supply to the Sabatier reactor. The positive slope portions are due to CO_2 concentrator desorption. As shown in Figure 2.1-2 when Bed No. 2 is absorbing, Bed No. 3 is desorbing. From the earlier discussion concerning steam desorption, it is apparent that during the initial portion of the desorption phase air in the bed is eluted and flows back to the cabin. The CO_2 zone is subsequently eluted and during this portion of the desorption phase flow is directed to the CO_2 accumulator. This results in the positive slopes shown for accumulator pressure changes in Figure 2.1-2. Following elution of CO_2, steam flows out of the bed and the effluent is again diverted back to the cabin via the condensing heat exchanger. During this portion of the desorption phase, the P_{CO_2} in the accumulator again decreases due to the demand of the Sabatier reactor.

2.1.3 Simulation of Concept

The simulation of this concept is performed by dividing the subsystem into functional components, suitably connecting the components, and incorporating interface and control logic into GP0LY. Figure 2.1-3 is a schematic for the G-189A components required for simulation of a typical subsystem. The subroutines used are shown in parenthesis on the figure.

Gas from the cabin is supplied to the subsystem by component 14 (ALTC0M). This flow is circulated by FAN component 4 to bypass valve 5 (SPLIT). The flow not bypassing goes to absorbing bed component 6 (C0S0RP). This component simulates a solid amine's bed which removes CO_2 from the cabin airstream. Since the bed is relatively wet with respect to the cabin air, moisture is picked up by the airstream. This moisture is removed by condensing heat exchanger component 7 (ANYHX). The coolant flow to this component is supplied by component 17 (ALTC0M). The dehumidified air then passes through a charcoal trap, component 8, which removes odors picked up in the amine's bed. The charcoal trap is simulated by subroutine ADS0RB.

While component 6 is removing CO_2 from the cabin airstream, component 16 (C0S0RP) is being purged with superheated steam to drive off CO_2 absorbed previously. Components 6 and 16 operate in a cyclic manner. While 6 is absorbing, 16 is desorbing. Steam to the bed is supplied by steam generator component 15. This component is simulated by a newly prepared subroutine SMGEN. Feed water to this component is pumped by metering pump 19 (PUMP) from water accumulator component 10 (TANKG). Condensate from heat exchanger components 7 and 12 is recirculated to this accumulator tank. Component 20 uses a new subroutine H2OSUM to sum up the flows from these two sources. Makeup water to the accumulator is supplied by feed water tank component 9 (TANKG).

The CO_2-steam mixture from the desorbing resin bed 16 is pumped by compressor 11 (FAN) through condensing heat exchanger component 12 (ANYHX). Coolant for this heat exchanger is supplied by component 18. De-humidified CO_2 from the heat exchanger is pumped to accumulator component 13 (TANKG).

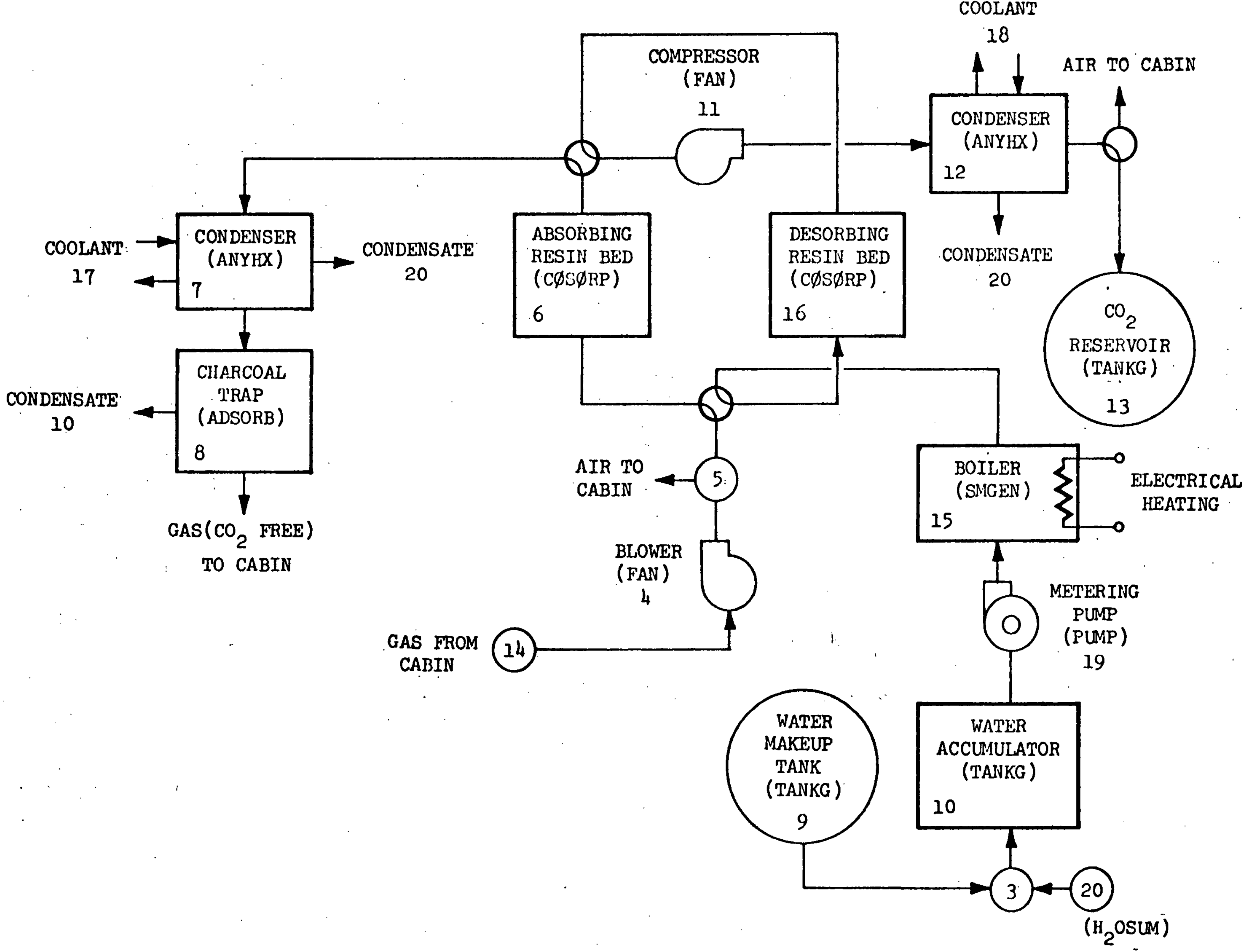


FIGURE 2.1-3 G189A SIMULATION OF A TYPICAL STEAM DESORBED SOLID AMINE CO_2 CONCENTRATOR

2.1.4 Sample Problem

Description -

A sample problem was prepared to demonstrate the simulation of the subsystem shown in Figure 2.1-3. The assumed inlet conditions of flow to the subsystem are based on requirements for a six-man EC/LS system. Logic has been incorporated into GPØLY to simulate valve sequencing operations which are required when switching the beds from an absorbing to disorbing mode.

Assumptions -

1. Gas from Cabin (Air)

   Flow: 19 scfm $\cong$ 84.6 lb/hr

   Relative Humidity = 48% $\simeq$ .00905 $\frac{\text{lb } H_2O}{\text{lb dry air}}$

   CO_2 partial pressure = 3.0 mmHg

   Temperature = 75°F

   Pressure = 14.7 psia

   Trace contaminates = .02 lb/hr

2. Absorbing/Desorbing Solid Amines Bed

   Length = 5.5 inches*

   Frontal area = 1.57 ft

   Bulk density = 28.8 lb/ft^3

   Pellet diameter = .00115 ft

   Pellet heat capacity (dry) = 0.26 Btu/lb°F

   Void fraction = 0.40

   Superficial surface area = 3130. ft^2/ft^3

   Heat of sorption for CO_2 = 250. Btu/lb

   Heat of sorption for H_2O = 1400. Btu/lb

   Heat transfer coefficient

   - during absorption : calculated by program
   - during desorption = 3.2 Btu/hr-ft^2-°F

---

* Effective length when dry.

Mass transfer coefficients (CO_2)

during absorption = 6.8×10^{-4} $\frac{\text{lb moles}}{\text{hr-ft}^2\text{-mmHg}}$

during desorption = 14.0×10^{-4} $\frac{\text{lb moles}}{\text{hr-ft}^2\text{-mmHg}}$

Mass transfer coefficients (H_2O)

during absorption = 6.8×10^{-6} $\frac{\text{lb moles}}{\text{hr-ft}^2\text{-mmHg}}$

during desorption = 22.0×10^{-4}

Initial conditions

during absorption:

CO_2 loading = .018 lb CO_2/lb dry resin

H_2O loading = 0.22 lb H_2O/lb dry resin

Bed temperatrue = 200°F

during desorption

CO_2 loading = 0.0310 lb CO_2/ lb dry resin

H_2O loading = 0.22

Bed temperature = 75°F

Operating conditions

duration of absorption cycle = 20 minutes

duration of desorption cycle = 20 minutes

3. Blower Characteristics

Heat dissipated into air = 60 watts

4. Air Condensing Heat Exchanger Characteristics

Coolant flow rate = 200. lb/hr

Coolant inlet temperature = 40.

Estimated overall thermal between gas and coolant = 50 Btu/hr°F

Heat exchanger time constant = 10 seconds

Coolant: Water

5. Water Makeup Tank Characteristics

Volume = 1.0 ft^3

Overall heat transfer conductance to surroundings = 1.0 Btu/hr °F

Initial volume = = 0.5 ft^3

Outside surface area = 1.0 ft^2

Pressure = 14.7 psia

Initial Mass in Tank = 31.2 lb

6. Water Accumulator

Volume = 0.15 ft^3

Overall heat transfer conductance to surroundings = 1.0 Btu/hr°F

Initial volume = 0.075 ft^3

Outside surface area = 1.00 ft^2

Initial mass in tank = 4.7 lb

7. Steam Generator (Boiler) Characteristics

Steam generation rate = 4.00 lb/hr

Temperature = 220°F

Pressure = 14.7 psia

8. Desorbing CO_2 Compressor Characteristics

Heat dissipated into gas stream = 10 watts

9. CO_2/Steam Mixture Condensing Heat Exchanger Characteristics

Coolant Type = water

Coolant flow rate = 200 lb/hr

Coolant inlet temperature = 40°F

Estimated overall thermal conductance between gas and coolant = 50 Btu/hr°F

10. CO_2 Accumulator Characteristics

Volume $= 2.0\ ft^3$

Overall heat transfer conductance to surroundings = 2. Btu/hr-°F

Initial pressure = 14.5 psia

CO_2 use rate = .575 lb/hr

Initial mass in tank = .307 lb

11. Water Metering Pump

Electrical input power = 15 watts

Pressure rise = 14.0 psi

Flow = 4.0 lb/hr

Special Notes —

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
    a. Bed length
    b. Frontal area
    c. Volumetric flow rate through bed
    d. Duration of absorption cycle

2. When attempting to match predicted results with experimental results for the same bed configuration and conditions, the following parameters should be varified:
    a. Pellet characteristics (effective diameter, particle density, superficial surface area, void fraction, etc.)
    b. Absorption isotherm data and heats of sorption.

2.2 VACUUM DESORBED SOLID AMINES

2.2.1 Process Description

This concept uses a solid amine resin bed to absorb CO_2 from a spacecraft atmosphere. The bed is regenerated at suitable time intervals by the combined effects of heat and vacuum. The CO_2 driven off in the bed is pumped to an accumulator for storage or usage by another subsystem. The accumulated gas may be dumped overboard or fed to an oxygen regeneration or propulsion system.

A prototype system using a proprietary resin designated as Gat-O-Sorb is described in reference 2.1. The reported advantages of this system are that no predrying of the gas is necessary prior to carbon dioxide absorption and only moderate regenerative conditions (180°F and 40 mmHg) are necessary. One possible disadvantage of this system is that a considerable amount of water is also carried off by the vacuum pumping system during desorption cycle. Reference 2.1 reported a weight ratio of between 0.1 and 0.5lb H_2O/lb CO_2 collected during desorption. In reference 1.2 it was reported that for vacuum desorbed IR-45 solid amine resin, water is desorbed ahead of CO_2. Here a 20% bed water content was necessary to obtain a 2% value of CO_2 bed loading. Thus, up to 10 lb H_2O may be desorbed/lb CO_2. This could pose a significant water removal problem.

Figure 2.2-1 shows a schematic of a prototype Gat-O-Sorb process. The unit was found to remove 0.41 lb CO_2/hr with a total resin weight of 30 lbs. The unit was tested through 91 different operating cycles without indication of absorbent deterioration.

The process shown in Figure 2.2-1 may be described as follows: CO_2 is removed from the process gas in one bed while absorbed CO_2 is being removed in the other bed. Two positions, four port valves are used to alternately reverse the bed functions. A centrifugal blower drives process gas through the absorbing bed, and a vacuum pump purges the desorbing bed. The beds are heated or cooled by tube-and-fin heat exchangers inside each canister

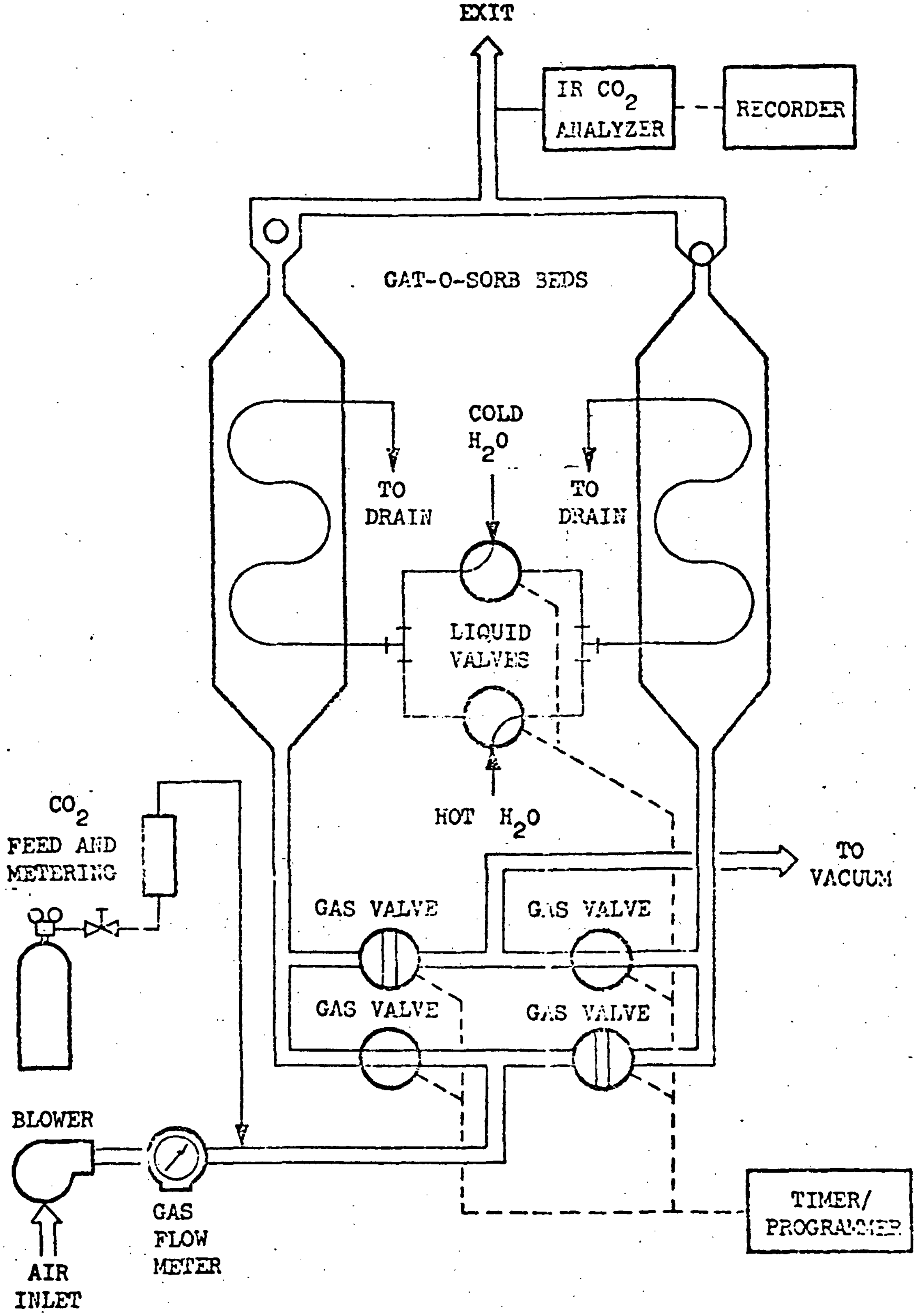


FIGURE 2.2-1 FLOW DIAGRAM OF BENCH SCALE GAT-O-SORB PROCESS

and in direct contact with the adsorbent particles. When absorbing, cool water is circulated through a bed. When desorbing, hot fluid is used.

Below inlet relative humidities of 50%, the absorbent was found to gradually dehydrate and lose its capacity for CO_2 absorption. RH above 50% was found not to be harmful to the process. RH below 50% could be tolerated for exposure times of several hours.

2.2.2 Simulation of Concept

The thermal/vacuum desorbed amines concept for CO_2 removal will be simulated by suitably connecting G-189A components which simulate individual components or functions of the concentrator. Figure 2.2-2 illustrates the G-189A components required for a typical subsystem. The subroutines used for each component are given in parenthesis.

Gas from the cabin is supplied by component 1 (ALTC0M). The gas is circulated to the subsystem by blower component 2 (FAN). The gas flows to component 3 (SPLIT) which controls the amount of gas bypassing the subsystem. Flow then passes through a solid amines resin bed where CO_2 is removed by absorption. Cooling fluid (water) flows from component 5 (ALTC0M) through the bed's integral heat exchanger. The coolant is required for removing the heat of absorption and the thermal energy stored in the bed during the thermal/vacuum desorption cycle. CO_2 free gas flows from the bed to charcoal trap component 7 (ADSORB) and back into the cabin.

While component 6 is absorbing CO_2, component 8 (VACDSP) is being desorbed of CO_2 collected previously. Desorption is affected by the combined effects of heat and vacuum. The heat is supplied by hot water from component 4. Desorbed CO_2 plus water vapor is transferred by vacuum pump component 9 (VACPMP) through condensing heat exchanger component 10 (ANYHX). Water vapor picked up during desorption is removed in this component. The dehumidified gas then flows to accumulator tank component 12 (TANKG) for storage or use by an oxygen regeneration subsystem.

2.2.3 Sample Problem

Description - A sample problem was set up for the subsystem shown in Figure 2.2-2. The inlet conditions selector are based on requirements for CO_2 removal for a six man system. The logic necessary to simulate time dependent operations such as valve sequencing is incorporated in GP0LY.

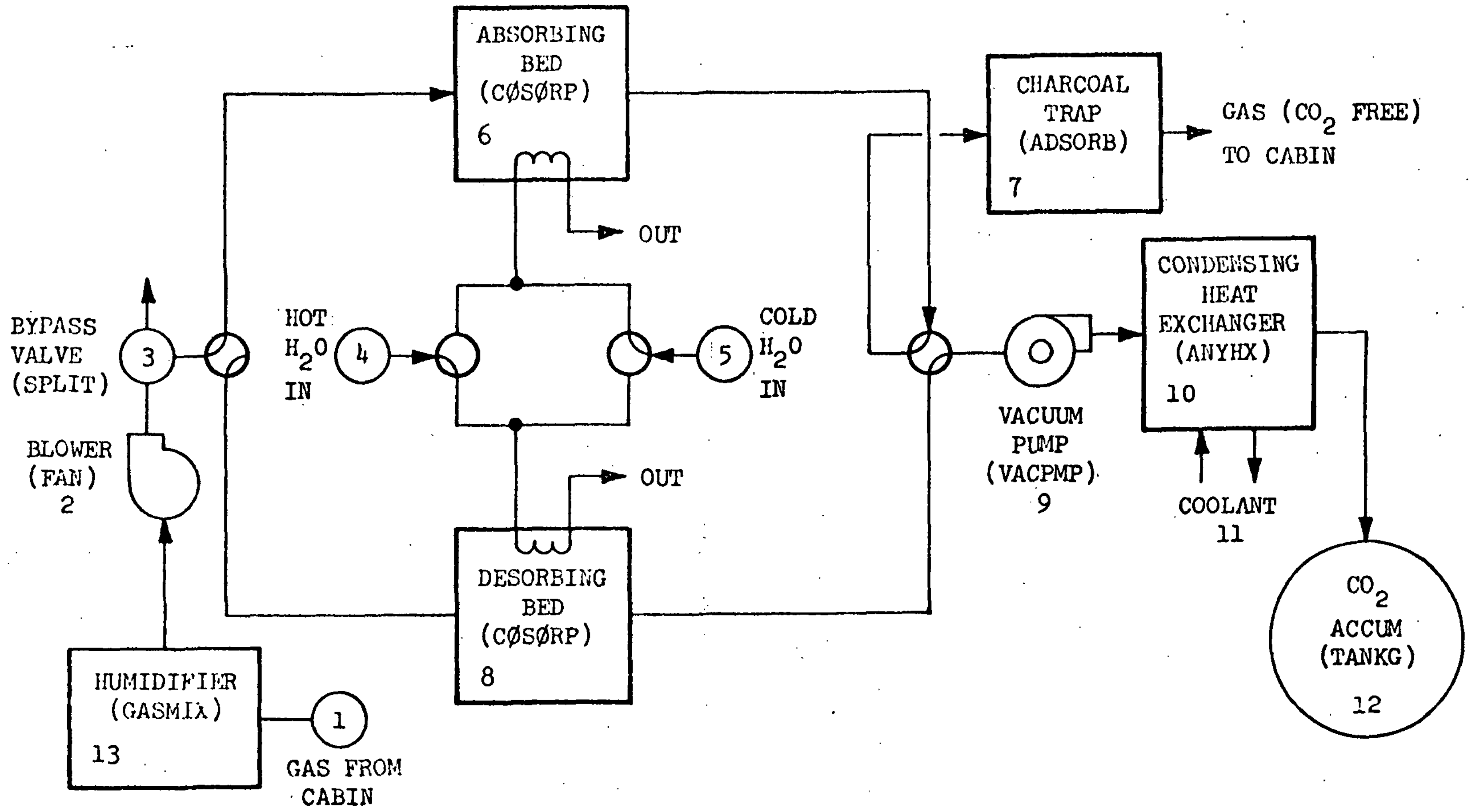


FIGURE 2.2-2 G189A SIMULATION OF VACUUM DESORBED AMINE BED

Assumptions -

1. Gas from Cabin (Air)

Flow

Dry-CO_2 free constituents =	83.6 lb/hr
CO_2	.507 lb/hr
H_2O vapor	.766 lb/hr
	84.873 lb/hr

Relative humidity = 50% ∿ .0094 lb H_2O/lb dry air

CO_2 partial pressure = 3.0 mm Hg

Temperature = 75°F

Pressure = 760 mm Hg

2. Absorbing/Desorbing Solid Amines Bed

Length = 5.5 inches*

Frontal area = 1.57 ft

Bulk density = 28.8 lb/ft^3

Pellet diameter = .00115 ft

Pellet heat capacity (dry) = 0.26 Btu/lb °F

Void fraction = 0.40

Superficial surface area = 3130 ft^2/ft^3

Heat of sorption for CO_2 = 250 Btu/lb

Heat of sorption for H_2O = 1400 Btu/lb

Mass transfer coefficients during absorption:

for CO_2 = 6.8×10^{-4} lb moles/hr-ft^2-mm Hg

for H_2O = 6.8×10^{-4} lb moles/hr-ft^2-mm Hg

Integral heat exchanger data

thermal capacitance of Hx = 0.208 Btu/°F

thermal capacitance of cooling fluid = 1.00 Btu/°F

---

* Effective length when dry.

Heat transfer coefficients during absorption:

gas to bed = (calculated by program)

gas to heat exchanger core = 0

bed to heat exchanger core = 146.0 Btu/hr-°F

heat exchanger core to bed = 146

Initial Conditions:

during absorption:

CO_2 loading = .018 lb CO_2/lb dry resin

H_2O loading = 0.22 lb H_2O/lb dry resin

Bed temperature = 180°F

during desorption:

CO_2 loading = 0.0310 lb CO_2/lb dry resin

H_2O loading = 0.22

Bed temperature = 75°F

Operating Conditions

duration of absorption cycle = 20 units

duration of desorption cycle = 20 minutes

Cooling Fluid Requirements (Water)

Flowrate = 270 lb/hr

Inlet Temperature = 55°F

Heating Fluid Requirements (Water)

Flowrate = 270 lb/hr

Inlet Temperature = 200 °F

3. Blower Characteristics

Heat dissipated into air = 60 watts

4. Desorbing Gas Condensing Heat Exchanger

Coolant type = water

Coolant inlet temperature = 40°F

Estimated thermal conductance between gas and coolant = 7.5

Flow rate cooling fluid = 10 lb/hr

5. Vacuum Pump Characteristics

Isentropic compression

$\eta_{aero} = 0.40$

$\eta_{motor} = 0.60$

K = polytropic exponent = 1.304 (CO_2 @ 15°C)

Flow determined from generalized curve for small vacuum pumps (see Figure 2.2-3).

6. CO_2 Accumulator Characteristics

Volume = 2.0 ft^3

Overall heat transfer conductance to surroundings = 2 Btu/hr-°F

Initial pressure = 20 psia

CO_2 use rate = .575 lb/hr

Initial mass = 0.307 lb

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
    a. Bed length
    b. Frontal area
    c. Volumetric flow rate through bed
    d. Duration of absorption cycle
2. When attempting to match predicted results with experimental results for the same best configuration and conditions, the following parameters should be varified:
    a. Pellet characteristics (effective diameter, particle density, superficial surface area, void fraction, etc.)
    b. Absorption isotherm data and heats of sorption.
    c. Heat transfer coefficients
    d. Mass transfer coefficients

3. The performance of the desorbing bed, vacuum pump, and accumulator are highly dependent on one another. When integrating a concentrator subsystem simulation into a larger or complete EC/LS simulation, it is suggested that the bed, vacuum pump, and accumulator be put in a subloop with a smaller computing interval than the overall system computing interval.

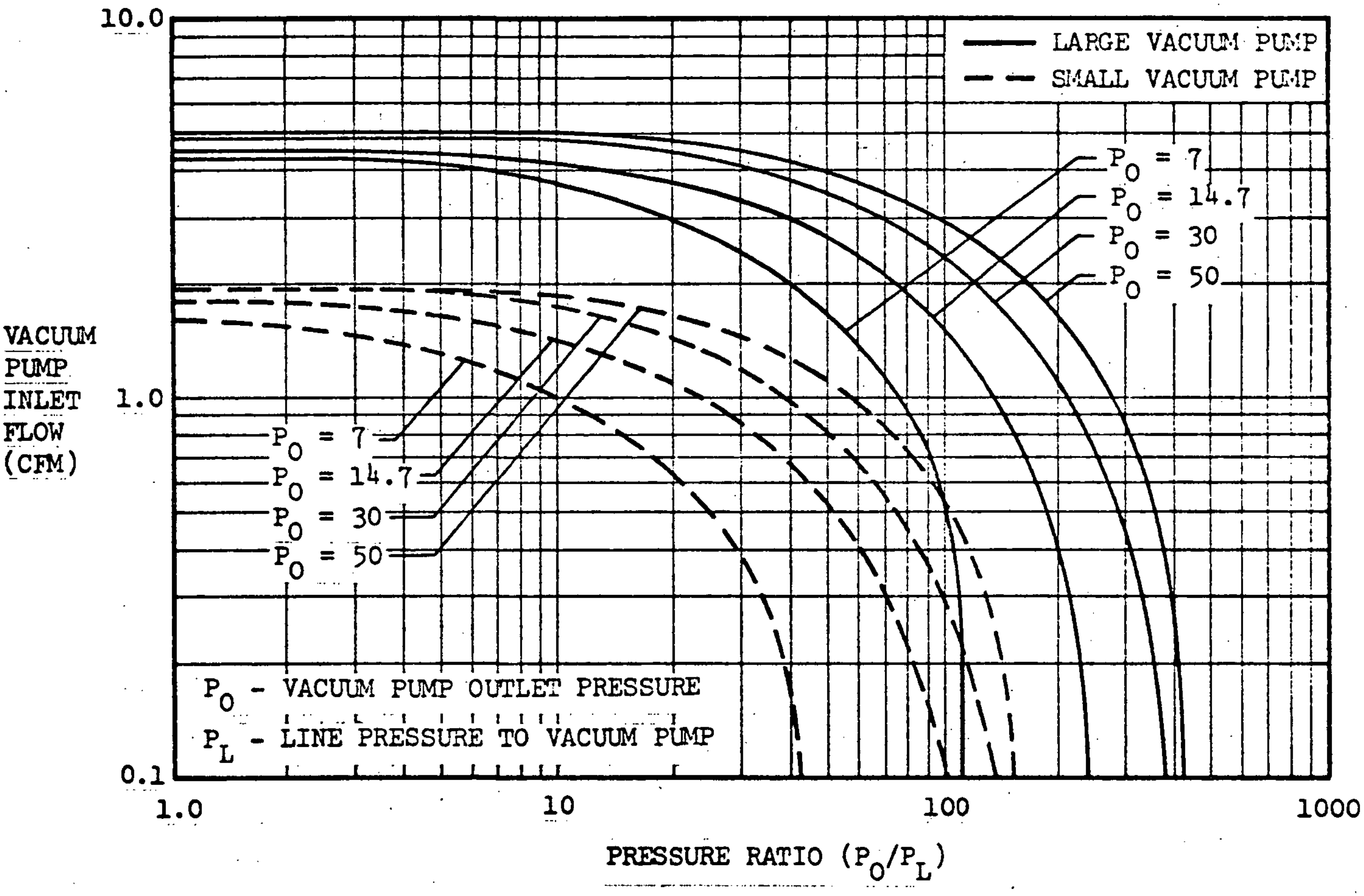


FIGURE 2.2-3 VACUUM PUMP CHARACTERISTICS

2.3 CARBONATION CELL

2.3.1 Process Description

The carbonation cell concentrator is an electrochemical device for collecting CO_2 from a cabin atmosphere. The process operates in a continuous rather than cyclic manner. The CO_2 collected is free of diluent gas contamination. Figure 2.3-1 illustrates the major components of a typical carbonation cell collector. Moist air is circulated into the cathode compartment of Stage I. An impressed voltage creates electrolytic reactions at the cell's two electrodes which are separated by an aqueous carbonate electrolyte held within an asbestos matrix. The net effect of the reactions is to liberate O_2 and CO_2 at the cell's anode compartment. Purity ranges between 50 and 70 mole percent. Air depleted in oxygen and with negligible amounts of CO_2 flows from the outlet of the cathode back to the cabin.

The gas freed at the anode is then transferred to Stage II which employs an aqueous acid electrolyte. An impressed voltage and accompanying electrolytic reactions create a liberation of only O_2 at the anode of this stage. CO_2 is concentrated at the cathode of this cell.

The concentrated CO_2 stream from the Stage II cathode passes through a condenser/separator to remove water vapor gained through evaporation in the cells. A compressor is used to force the CO_2 into a storage tank. Details on the operation of the I and II stages of the concentrator, which were abstracted from reference 3.1, are given below:

<u>First Stage (Carbonation Cell) Operation</u> -

Process air flows into the cell cathode compartment where O_2 and CO_2 are absorbed by the cell electrolyte. Oxygen combines with water to form hydroxyl ions while CO_2 reacts with hydroxyl ions to form carbonate ($CO_3^=$) or bicarbonate (HCO_3^-) ions. The $\overline{OH}$, $CO_3^=$, and HCO_3^- ions diffuse through the electrolyte to the anode compartment. These ions react at the anode to liberate CO_2 and H_2O. Figure 2.3-2 illustrates the electrochemical reactions at the anode and cathodes.

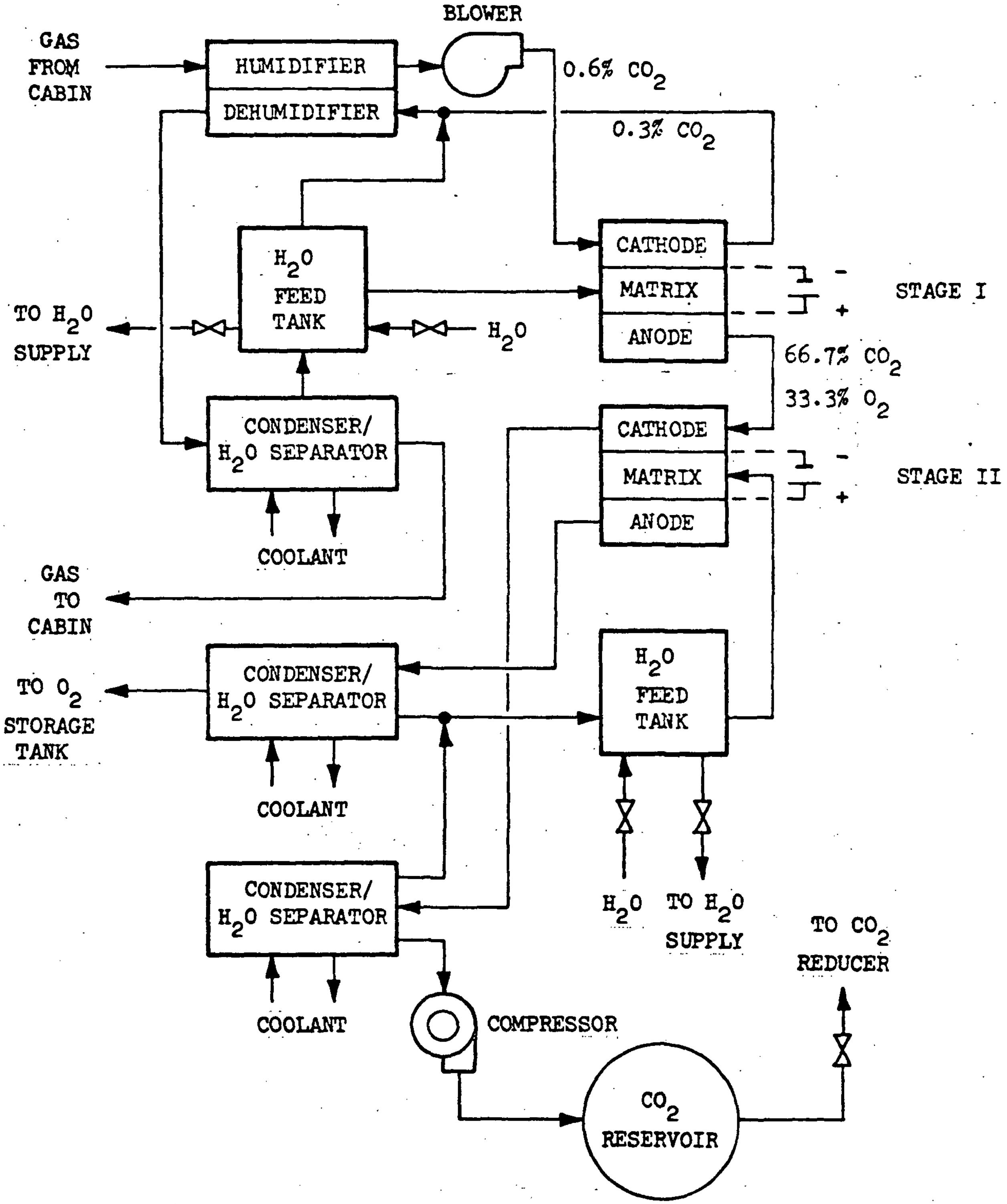


FIGURE 2.3-1 CARBONATION CELL CO_2 COLLECTOR

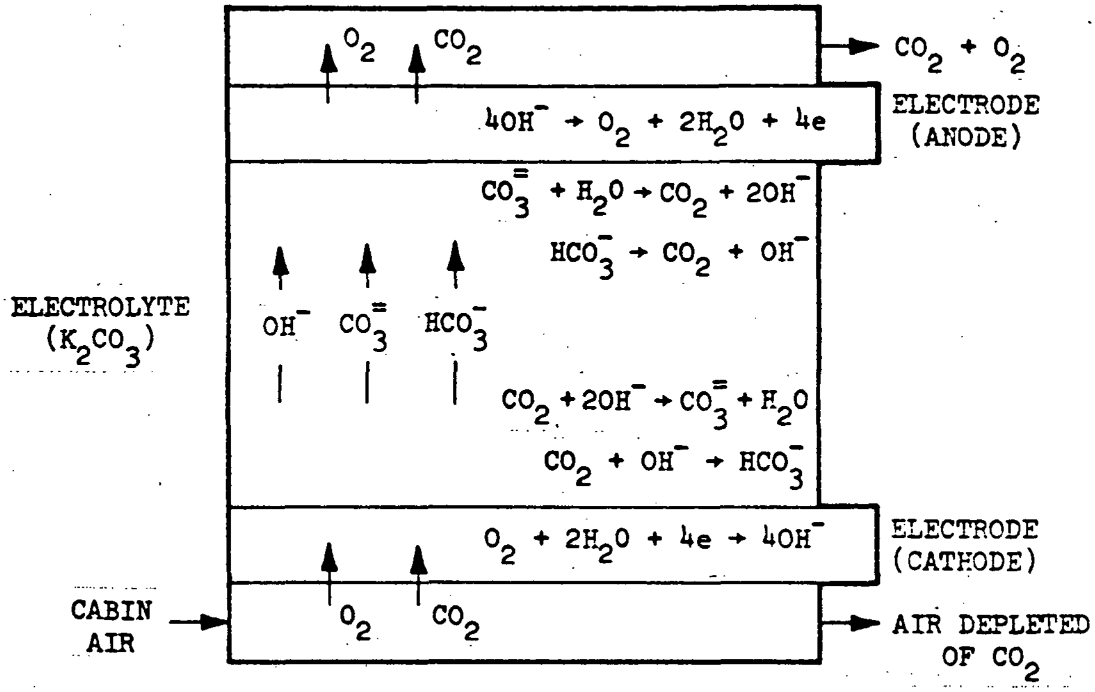


FIGURE 2.3-2 STAGE 1 CELL-SCHEMATIC REPRESENTATION

The electrochemical reactions vary significantly with carbon dioxide partial pressure in the cathode gas. For very low CO_2 concentrations, only $\overline{OH}$ ions are formed and thus only O_2 is liberated at the anode. At very high CO_2 partial pressures, a large number of bicarbonate ions are formed to favor a high CO_2 to oxygen ratio at the anode. At normal operating levels of 0.03 to 1.0% CO_2, most of the carbon dioxide is liberated through transference by the carbonate ions. The effect of CO_2 cathode partial pressure is illustrated by figure 3.2-3.

Typical performance curves for a cell operating at 10 psia are shown in Figures 2.3-4 and 2.3-5. At a current density of 40 amps/ft^2 and a cell temperature of 140°, the CO_2 transfer rate is approximately 5cc per amp-min. The anode gas concentration is over 55% CO_2.

Second Stage Operation -

CO_2 level could be boosted to a maximum amount of 80% through use of a second carbonate stage (see Figure 2.3-3). A second stage employing an acid electrolyte was found effective in achieving a CO_2 concentration of almost 100%. Here the active species is the hydrogen ion. Oxygen reacts with this ion at the cell cathode to form water which migrates to the anode. Here the water is decomposed to oxygen and hydrogen ions. Thus no CO_2 is transferred in this stage and a high separation efficiency is achieved. Details on the cell reactions are shown in Figure 2.3-6. Figure 2.3-7 shows the cell terminal voltage as a function of current density. Using a design value of 50 amps/ft^2 oxygen was found to be transferred at a rate close to the theoretical value of 3.5cc(STP) per amp-min.

2.3.2 Simulation of Concept

The simulation of the carbonation cell CO_2 concentration subsystem is performed by dividing the subsystem into major functional components which are modeled by G-189A component subroutines. Figure 2.3-8 represents a typical subsystem. Process gas flow from the cabin is supplied by component 1(ALTC0M).

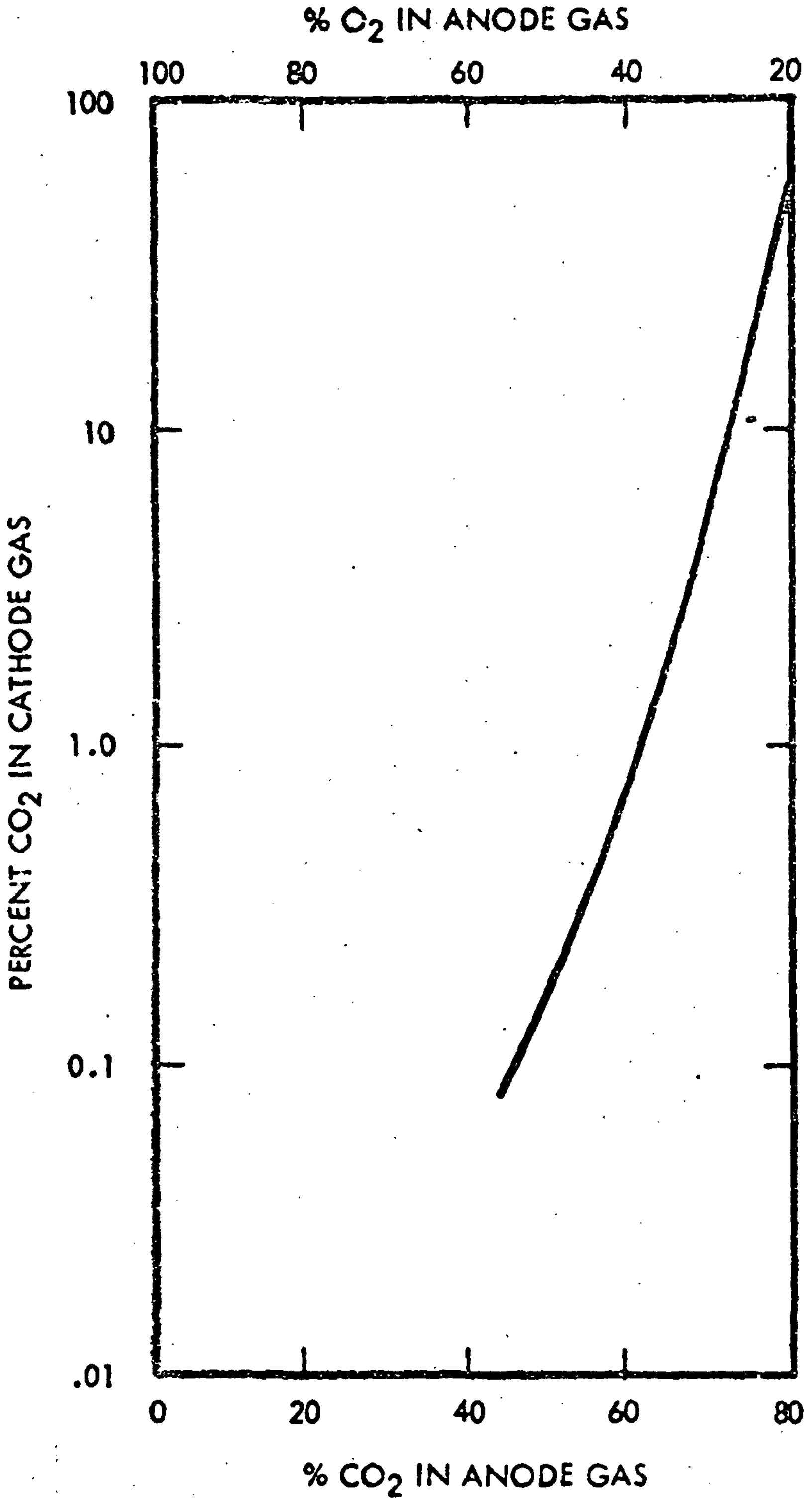


FIGURE 2.3-3 ANODE GAS MIXTURE AS FUNCTION OF CATHODE GAS MIXTURE FOR CARBONATION CELL

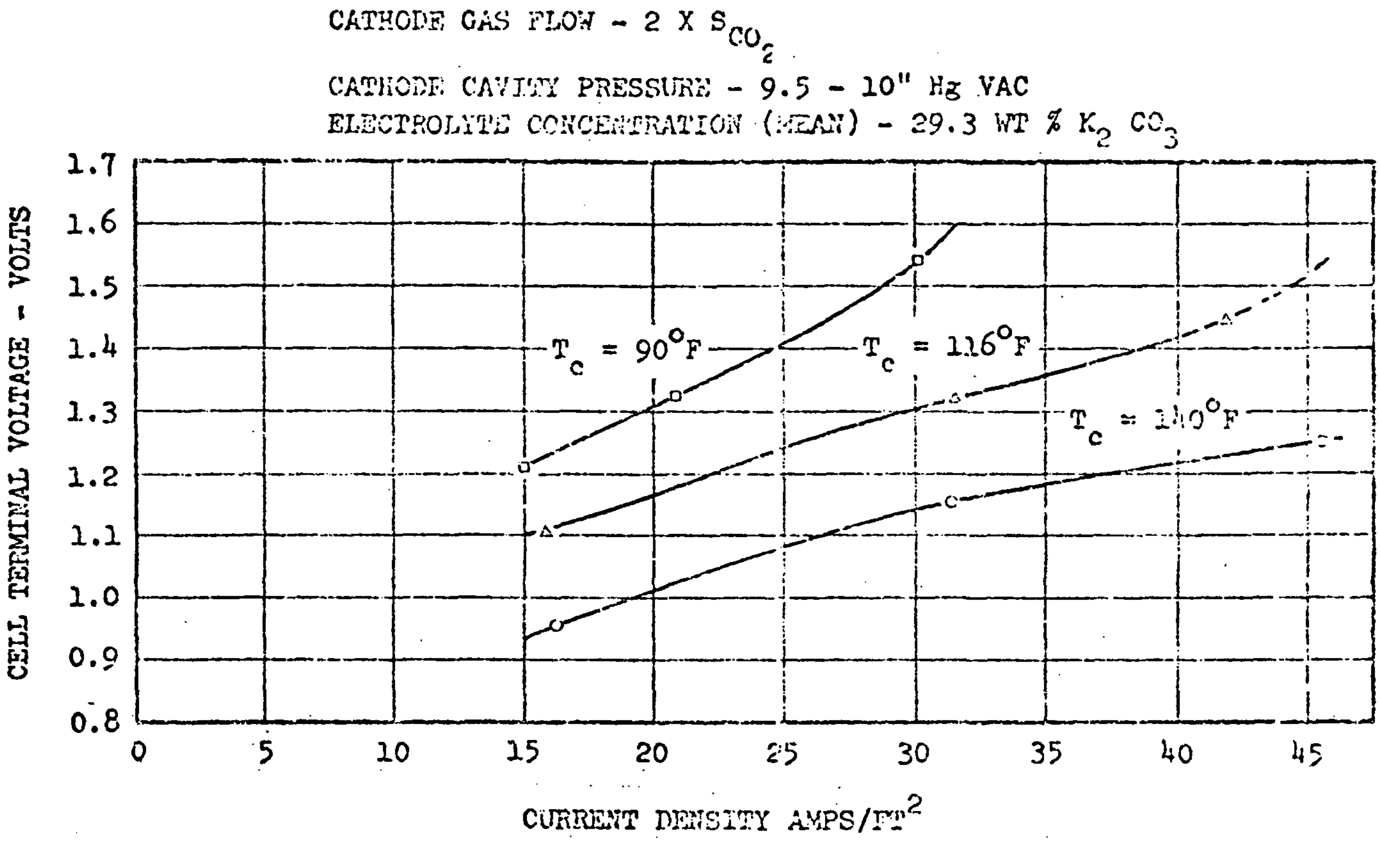


FIGURE 2.3-4 CELL VOLTAGE AS FUNCTION OF CELL CURRENT - STAGE I

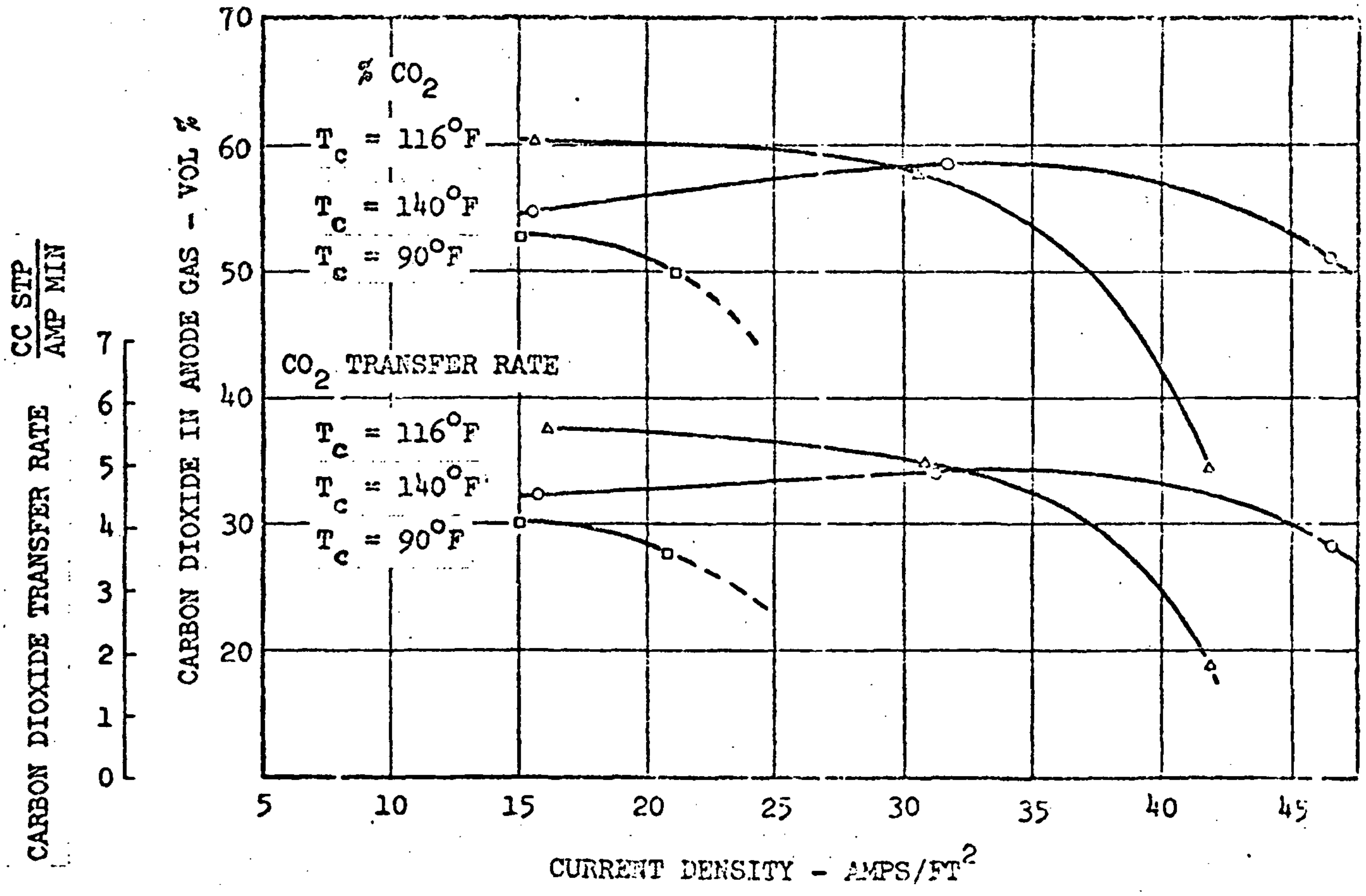


FIGURE 2.3-5. CARBON DIOXIDE TRANSFER AS FUNCTION
OF CELL CURRENT - STAGE I

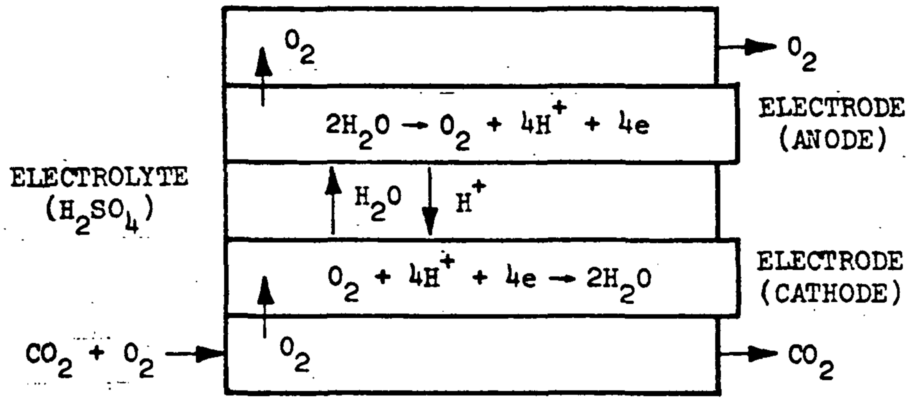


FIGURE 2.3-6 STAGE II CELL-SCHEMATIC REPRESENTATION

ACTIVE ELECTRODE AREA - 0.83 FT^2
CATHODE GAS FLOW - 1.3 x S_{O_2}

ELECTROLYTE CHARGE CONCENTRATION - 38.25 WT% H_2SO_4

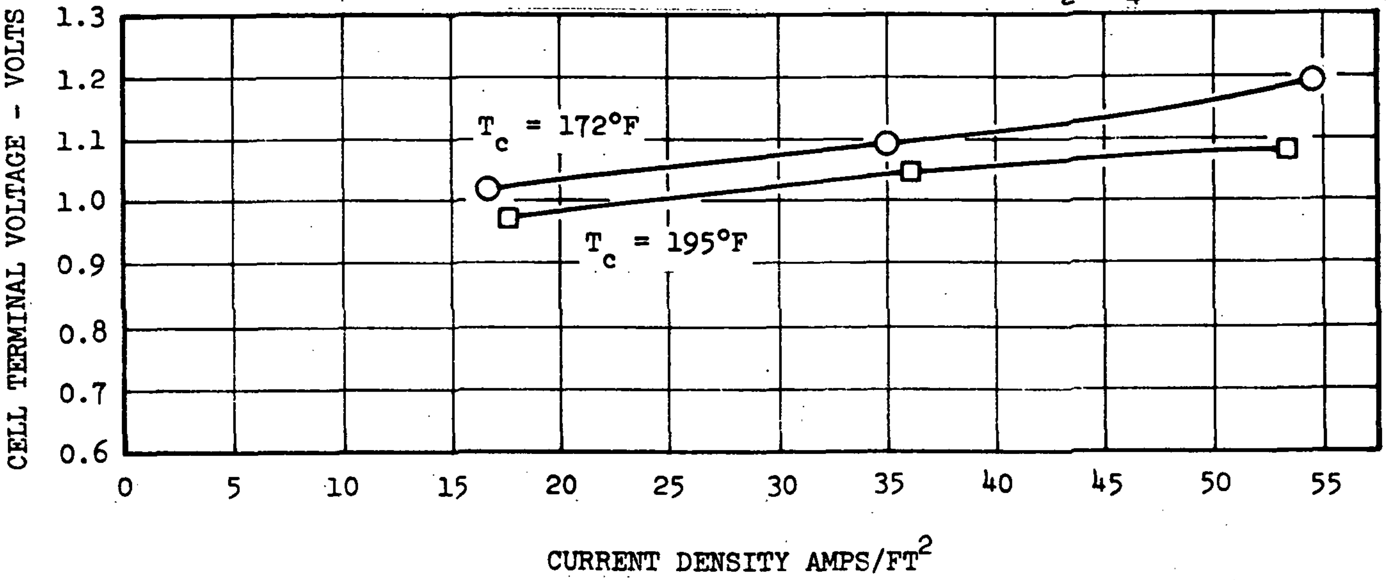


FIGURE 2.3-7 CELL VOLTAGE AS FUNCTION OF CELL CURRENT - STAGE II

A blower (FAN), component 2, forces process gas through the subsystem. Prior to entering the concentrator, the process gas flows through a humidifier (HUMID), component 3, where water vapor exchange takes place with the process gas leaving the first stage of the concentrator. The humidified process gas then flows to the cathode compartment of the first stage, component 4 (CARCL1), of the subsystem. Process gas leaves the cathode compartment essentially free of CO_2. An O_2/CO_2 mixture leaves the anode compartment. The purified process gas leaving the first stage flows back through component 3 (HUMIDT) to condenser/separator component 6(ANYHX) prior to returning to the cabin.

The CO_2/O_2 mixture from the anode compartment of the first stage flows to the cathode side of component 8(CARCL2) which is the second stage of the concentrator. CO_2 is obtained from the cathode side of this stage while O_2 is obtained at the anode side. CO_2 from the cathode side flows to condenser/water separator component 9(ANYHX). The dehumidified CO_2 is pumped by component 20(FAN) to a CO_2 reservoir component 21(TANKG). O_2 collected at the anode side of the second stage flows to condenser/water separator component 10(ANYHX). The dehumidified O_2 is pumped by component 22(FAN) to accumulator component 23(TANKG).

The condensate flows from condenser/water separator components 6, 9, and 10 are summed up by component 16(H20SUM). The total condensate flow is pumped by component 17(PUMP) to water storage tank component 18(TANKG). This tank provides makeup feed for the two carbonation cell stages, components 4 and 8. The amount of makeup water required is calculated by GP0LY logic. This water is added to the subsystem at component 5(GASMIX).

2.3.3 Sample Problem

Description —

The sample problem described here was prepared to verify the computational accuracy of the subroutines used for the carbonation cell concept. The subsystem, which is assumed to be sized for six men, is shown schematically in

Figure 2.3-8. Many of the values of input data are based on values reported in Reference 3.2.

Assumptions -

1. The conditions of the cabin air used in defining the data for component 1 are as follows:

Dry bulb temperature, °F	70.
Wet bulb temperature, °F	60.
Cabin pressure, psi	14.7
Partial Pressure CO_2, mm Hg	3.0
O_2 pressure, psia	3.1
CO_2 generation rate/removal rate per man	.1 lb/hr-man
Number of men	6

Reference 3.2 was used to provide data for determining the operating conditions, removal efficiency, and power requirements for the 6-man CO_2 concentrator subsystem. The removal efficiency of CO_2 of gas stream flowing through the concentrator system is ∿ 46%, which is used in calculating the input data to component 1.

Total air flow, lb/hr	211.987
Temperature, °F	70.0
Upstream duct outlet pressure, psi	14.7
Component outlet pressure, psi	14.7
Non-condensable flow, lb/hr	209.697
H_2O vapor flow, lb/hr	2.29
Non-condensable specific heat, Btu/lb-°F	.24
Non-condensable molecular weight, lb/mole	28.97
Oxygen flow, lb/hr	49.3
Diluent flow (N_2), lb/hr	159.13
Carbon dioxide flow, lb/hr	1.267

2. Blower Characteristics

Heat dissipated into process gas, watts	150

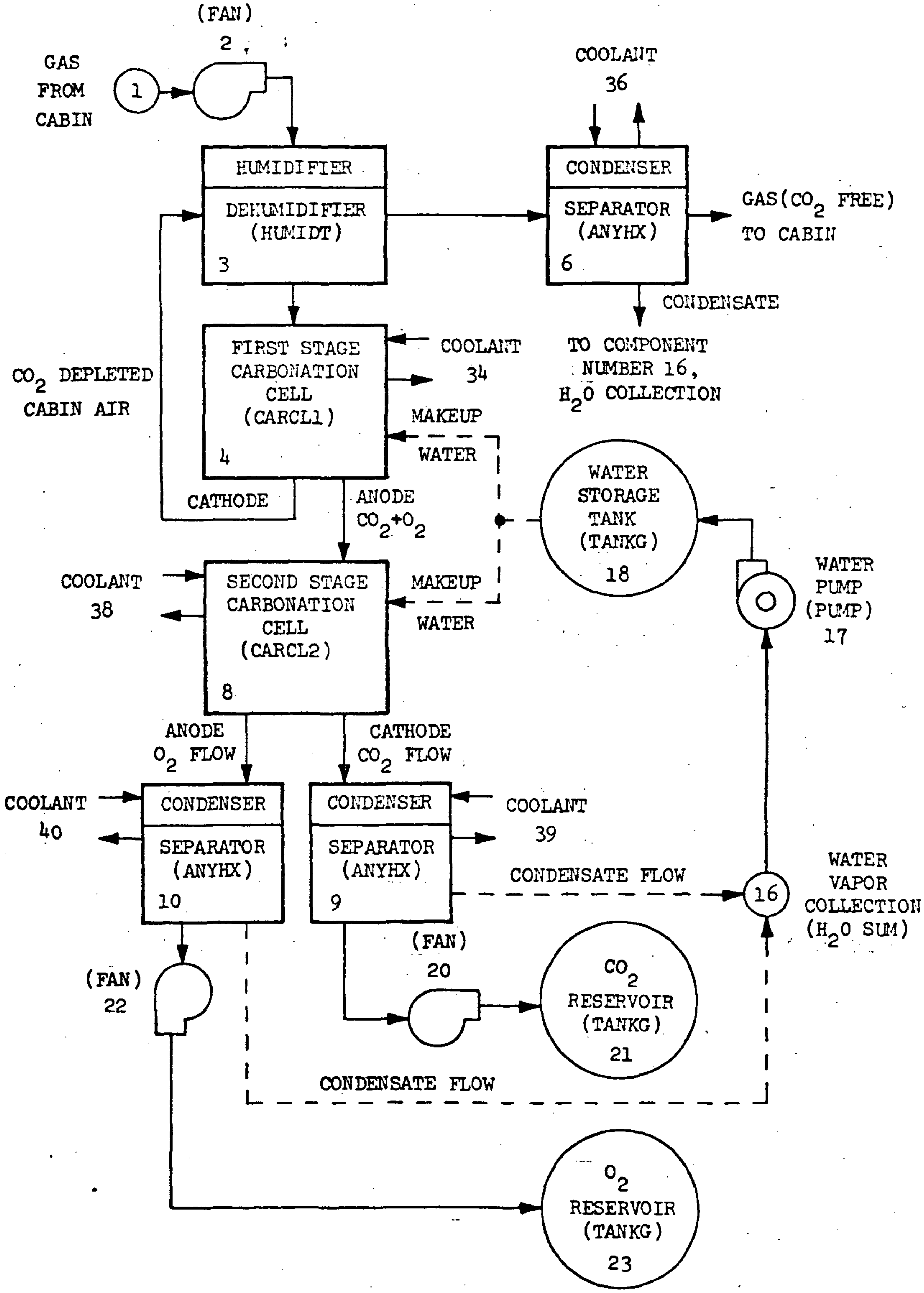


FIGURE 2.3-8 G189A CARBONATION CELL COMPONENT CONNECTION AND DEFINITION

3. Humidifier Characteristics

Mass transfer effectiveness = 95%

Heat transfer effectiveness = 94%

4. First Stage of Carbonation Cell Characteristics

Heat Loss Data:

Ambient gas temperature (°F)	70.
Thermal conductance between surface and ambient (Btu/hr-°F)	.1
Ambient wall temperature (°F)	60.
FA factor for radiation conductance (Ft^2)	2.
Structure temperature for heat short, (°F)	60.
Thermal conductance between module and structure (Btu/hr-°F)	.1

Cell Parameters:

Transfer rate of CO_2 (lb/hr-amp-cell)	.00121
Desired module temperature (°F)	140.
Heater turn-off temperature (°F)	138.
Actual temperature of module (°F)	140.
Design current density (amp/Ft^2)	35.
Area of cell (Ft^2)	1.0
Number of cells in the module	15
Voltage per cell	1.17
Relative humidity in exit cathode gasses (decimal fraction)	.48
Relative humidity in exit anode gasses (decimal fraction)	.95
Weight of water per cell in matrix (lb)	1.5
Weight of C_sCO_3 per cell in matrix (lb)	1.83
Desired solids concentration in matrix (%)	55.
Actual solids concentrator in matrix (%)	55.
Total pressure of stage (psia)	14.6
Thermal capacitance of stage (Btu/°F)	40.
Heat transfer conductance from coolant to cell (Btu/hr-°F-Cell)	33.

Component 34 provides the coolant flow to the first stage carbonation cell. The flow rate, pressure and temperature of the coolant flowing to the first stage are defined as follows:

Flow rate (lb/hr)	100.0
Temperature (°F)	100.0
Pressure (psia)	20.0

The physical properties of the coolant (water) listed below also apply to coolant provided by components 36, 38, 39 and 40.

Specific heat (Btu/lb-°F)	1.0
Density (lb/ft^3)	62.4
Viscosity (lb/hr-ft)	3.6
Molecular weight (lb/mole)	18.0
Conductivity (Btu/hr-ft-°F)	.325

Makeup water that is added to the first stage carbonation cell is provided by component 18, Water Storage Tank. The amount of makeup water required is computed by subroutine CARCL1 and is used through GP0LY logic to compute the outlet flow from the H_2O supply tank. A similar approach is used in modeling the water flow to the second stage carbonation cell, component 8.

5. Process Gas Condenser/Water Separator Characteristics

Overall UA (Btu/hr-°F)	35.
(NTU)Max	5.0
Primary side design outlet temp. (°F)	65.
Tolerance for design temperature (°F)	3.

The coolant to the heat exchanger is provided by component 36. The values of the parameters defining the inlet conditions are:

Flow rate (lb/hr)	40.0
Temperature (°F)	45.0
Pressure (psia)	20.

The physical properties of the coolant are the same as those defined for component 34.

6. Second Stage of Carbonation Cell Characteristics

Heat Loss Data:

Ambient gas temperature (°F)	70.
Thermal conductance between surface and ambient (Btu/hr-°F)	.1
Radiation wall temperature (°F)	60.
FA factor for radiation conductance (Ft^2)	2.
Structural temperature for heat short (°F)	60.
Conductance between module and structure (Btu/hr-°F)	.1

Cell Parameters:

O_2 removal efficiency	.98
Desired module temperature (°F)	172.
Heater turn-off temperature (°F)	174.
Heater turn-on temperature (°F)	170.
Actual temperature of the module (°F)	172.
Design current density (amp/Ft^2)	50.
Number of cells	8.0
Voltage per cell	125.
Relative humidity in exit cathode gas	.35
Relative humidity in exit anode gas	.95
Weight of H_2O per cell in matrix (lb)	2.
Weight of H_2SO_4 per cell in matrix (lb)	1.2
Desired H_2SO_4 concentration (%)	50.
Actual H_2SO_4 concentration (%)	50.
Vapor pressure of water over electrolyte (psi)	6.0
Total pressure of stage (psi)	14.7
Thermal capacitance of stage (Btu/°F)	45.
Heat transfer conductance from coolant to cell (Btu/hr-°F)	20.

The coolant flow to component 8 is provided by component 38. The flow rate, pressure, and temperature at the inlet are as follows:

Flow rate (lb/hr)	100.
Temperature (°F)	100.
Pressure, upstream duct (psi)	20.
Pressure, component outlet (psi)	20.

The makeup water to the second stage carbonation cell is provided by component 18.

7. CO_2/Water Separator Characteristics

Overall UA (Btu/hr-°F)	1.5
NTU (max)	5.
Design outlet temperature (°F)	45.
Tolerance in outlet temperature (°F)	5.

The coolant is provided by component 39. The flow, temperature and pressure are given as follows:

Coolant flow rate (lb/hr)	20.
Coolant temperature (°F)	40.
Coolant pressure, component outlet (psi)	20.
Coolant pressure, upstream duct (psi)	20.

8. O_2/Water Separator Characteristics

Overall UA (Btu/hr-°F)	3.0
NTU (Max)	6.0
Design primary outlet temperature (°F)	45.
Tolerance for design temperature (°F)	5.0

The coolant flow to the O_2/H_2O separator is provided by component 40. The flow rate, temperature, and pressure are:

Coolant flow rate (lb/hr)	10.
Temperature (^{o}F)	40.
Pressure, upstream duct (psi)	20.
Pressure, component (psi)	20.

9. The CO_2 and O_2 Reservoir Characteristics

	Component 21	Component 23
Ambient gas temperature (^{o}F)	70.	70.
Thermal conductance between surface and ambient (Btu/hr-^{o}F)	.05	.05
Ambient wall temperature (^{o}F)	60.	60.
Radiation FA factor (ft^2)	6.	6.
Structure temperature (^{o}F)	60.	60.
Conductance between tank wall and structure (Btu/hr-^{o}F)	2.2	2.2
Thermal capacitance of tank (Btu/^{o}F)	2.5	2.5
Conductance between fluid and wall (Btu/hr-^{o}F)	0.5	0.5
Total gas weight in tank (lb)	.076	.0555
Gas temperature in tank (^{o}F)	80.	80.
Tank volume (ft^3)	1.0	1.0
Tank pressure (psi)	10.0	10.0
Weight of non-condensable (lb)	.076	.0555
Specific heat (Btu/lb-^{o}F)	.205	.217
Molecular weight (lb/mole)	44.0	32.
Weight of CO_2 in tank (lb)	.076	0.0
Weight of O_2 in tank (lb)	0.0	0.555

10. Water Storage Tank Characteristics

Ambient wall temperature (°F)	70.
Conductance between ambient and surface of tank (Btu/hr-°F)	.1
Ambient wall and structure temperature (°F)	60.
Radiation FA factor (ft^2)	6.
Conductance structure to tank (Btu/hr-°F)	.1
Thermal capacitance (Btu/°F)	2.5
H_2O weight in tank (lb)	100.
Temperature (°F)	70.
Volume (ft^3)	2.5
Specific heat (Btu/lb)	1.0

The outflow from the water storage tank which is computed by GP0LY1 is set equal to the sum of the water requirements for components 25, 4, and 8.

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired rate, the following parameters may be varied to achieve the desired result:
   a. number of cells
   b. desired operating temperatures
   c. total current
   d. area of cells

2. When attempting to match predicted results with experimental results for the same unit configuration and conditions, the following parameters should be varified:
   a. CO_2 transfer rate as a function of current density and operating temperature
   b. Cell voltage and current
   c. Cell dimensions
   d. Heat transfer characteristics
   e. Electrolyte vapor pressure relationship

2.4 HYDROGEN DEPOLARIZED CELL

2.4.1 Concept Description

The hydrogen depolarized cell is an electrolytic process for CO_2 concentration. The concept evolved from the carbonation cell concept. The process differs in that only one stage is required, and that hydrogen is introduced at the anode of the cell. The hydrogen serves to depolarize the cell to shift the chemical equilibrium in the direction of CO_2 formation. The cell acts similar to a fuel cell since hydrogen and oxygen are consumed and electricity is generated. The electricity generated provides the energy required to create the electrolytic reactions which cause the separation of CO_2 from O_2. A considerable amount of design effort and development testing have been conducted for the concept over the past seven years (1965-1972).

The process has a considerable amount of flexibility in the range of CO_2 partial pressures over which it can operate. The removal rate can be modulated if desired. The unit operates continuously requiring no regeneration. In addition the unit is reported to have a low equivalent weight compared to the other concepts for CO_2 removal (Reference 4.2)

Figure 2.4-1 illustrates the reactions occurring in the cell. CS_2CO_3 electrolyte is used rather than the K_2CO_3 used in the carbonation cell. Moist cabin air is fed to the cathode where oxygen reacts to form $O\bar{H}$ ion. These ion react with CO_2 to form carbonate ions. The air leaving the cathode compartment thus is depleted in both O_2 and CO_2. The $CO_3^=$ ion migrate in the electrolyte to the anode where they react with water to generate CO_2. Hydrogen introduced at the anode reacts with $O\bar{H}$ ion to shift the anode reactions in the direction favoring formation of CO_2.

The CO_2 liberated at the anode is free of O_2 but mixed with H_2. The cell can operate effectively with percentages of H_2 varying from 20 to 90%. This mixture can be controlled to achieve the mix ratio desired for feed to a Sabatier CO_2 reduction process.

The concept incorporates an integral dehumidifier/humidifier to prevent dry out of the cells. Figure 2.4-2 shows a cross section of a typical cell. Further details on the operation of the cell are given in reference 4.2. Other information is provided in references 4.4, 4.5, 4.8. A detailed analytical model for the cell reactions is described in reference 4.12.

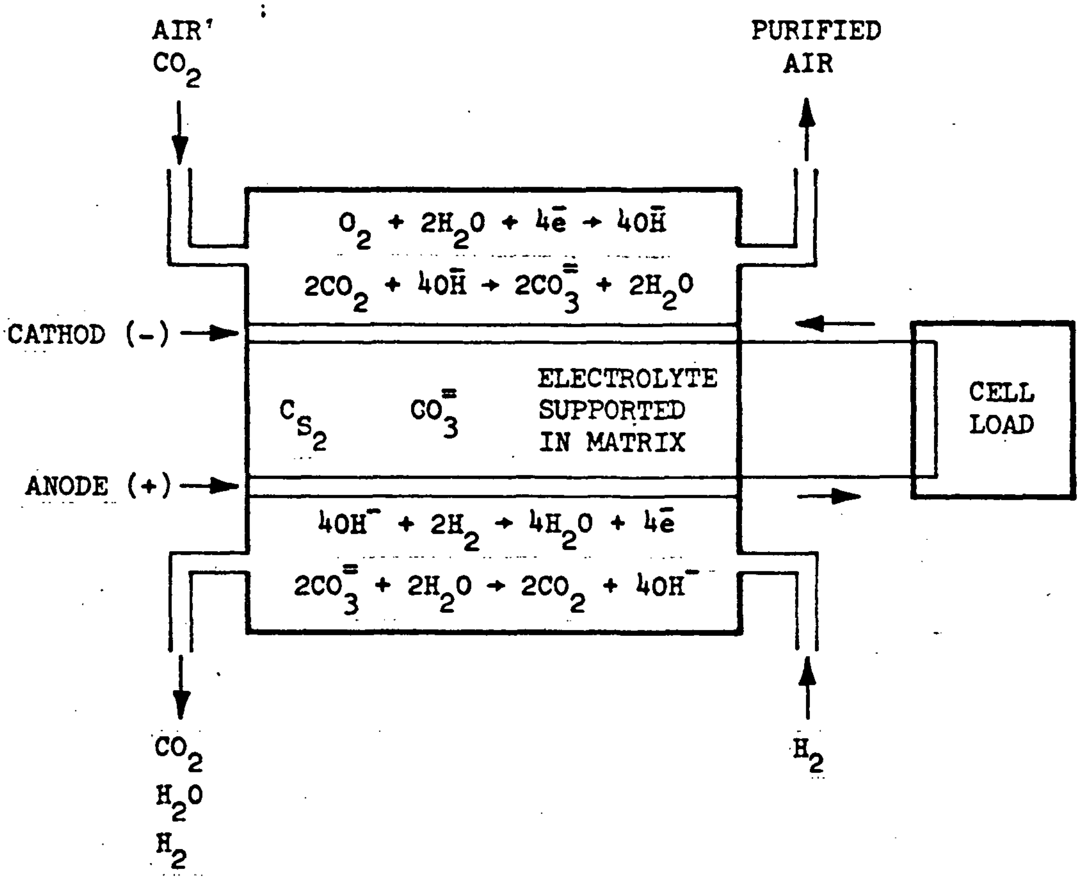


FIGURE 2.4-1 HYDROGEN DEPOLARIZED CELL

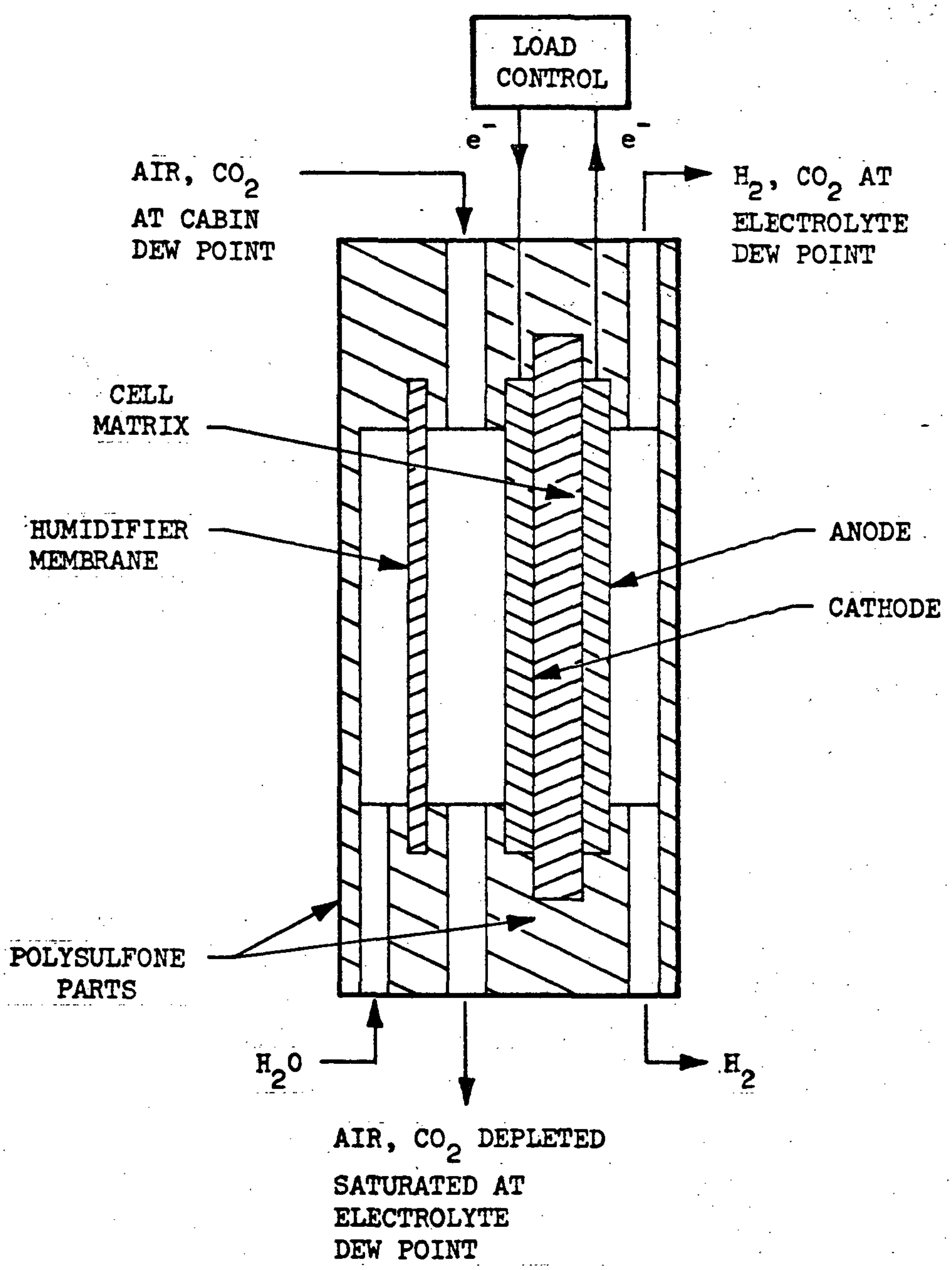


FIGURE 2.4-2 CELL SCHEMATIC

Thermal control of the cell temperature is accomplished through evaporation of water into the product streams.

2.4.2 Simulation of Concept

Figure 2.4.3 illustrates the functional components required for simulating the SSP Concentrator (Reference 4.1). The functions of each component are described as follows:

Air from the cabin is drawn through a dehumidifier component 2 (ANYHX). The dehumidifier is necessary to control air relative humidity within specified bounds. This control is necessary to prevent flooding or drying out of the cell electrolyte. The air then is drawn by blower component 3 (FAN) into the cathode compartment of hydrogen depolarized cell component 5 (H2DPØL). Here the CO_2 is scrubbed out by electrochemical reactions. The purified gas leaves the cell, flows through filter component 7 (ADSORB) which removes trace contaminants and returns to the cabin.

Hydrogen flow to the anode compartment is supplied by storage tank component 8 (TANKG). The hydrogen passes through filter component 9 (ADSORB) prior to entering the cell. In the anode compartment, hydrogen reacts with $\overline{OH}$ to generate water. The water reacts with $CO_3^=$ ions to regenerate CO_2. CO_2 and unreacted H_2 flow out of this compartment into storage tank component 10 (TANKG). This tank serves as a source of flow to a Sabatier reactor oxygen regeneration subsystem.

2.4.3 Sample Problem

<u>Description</u> -

A sample problem was prepared for the SSP subsystem previously described in Figure 2.4-3. A six-man sybsystem has been assumed. Data from reference 4.1 was used in preparing the sample problem.

<u>Assumptions</u> -

1. Flow of gas from cabin

   Flow

Dry CO_2 free constituents	984.	lb/hr
CO_2	5.97	lb/hr
Water vapor	9.4	lb/hr

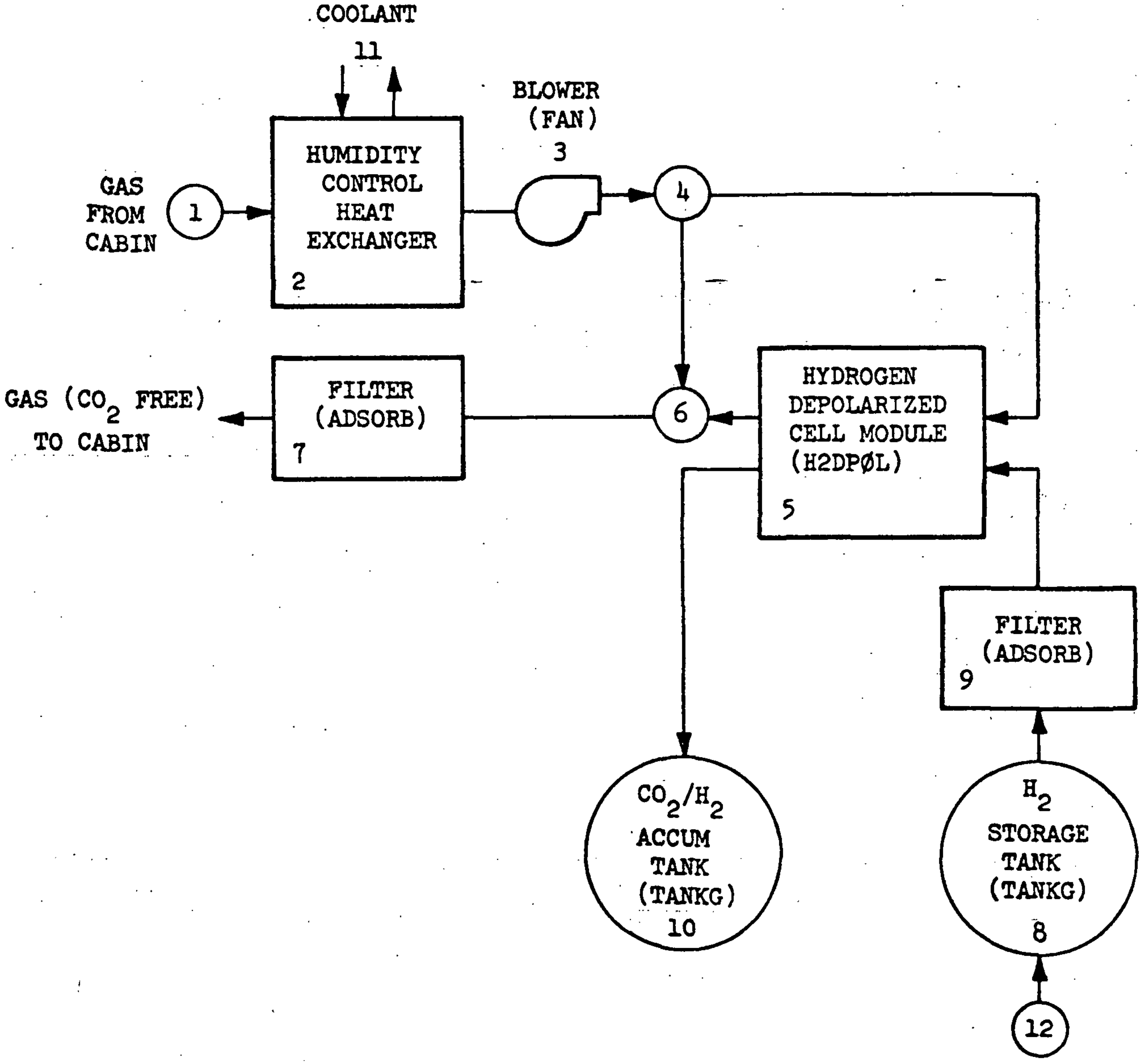


FIGURE 2.4-3 G-189A SIMULATION HYDROGEN DEPOLARIZED CELL CONCENTRATOR

Relative humidity = 50%

CO_2 partial pressure = 3.0 mmHg

Temperature = 75°F

Pressure = 760 mmHg

2. Dehumidifier Characteristics

Type of coolant = water

Coolant inlet temperature = 40°F

Coolant flow rate = 150 lb/hr

Desired dewpoint for air = 40°F

Heat exchanger effectiveness = 0.95

3. Subsystem Blower Characteristics

Heat dissipated into process gas = 20 watts

4. Hydrogen Depolarized Cell

Maximum CO_2 partial pressure in cabin = 3.0 mmHg

Cell temperature at time zero = 62.0°F

Lowest air temperature for operation = 52.0°F

Maximum air pressure for operation = 14.7 psia

Maximum air flow for operation = 200 ft^3/min

Maximum partial pressure of water vapor in air = 7.925 mmHg

Cell length = 0.5 ft

Total width of all cells = 54 ft

Air channel dimensions = 0.2 inches

Current collector width = 0.05 inches

Electrode spacing = 25 mils

Matrix thickness before compression = 60 mils

Matrix void volume fraction (dimensionless) = 0.70

Total mass of cell stack = 111. lb

Average specific heat of cell stack = 0.125 Btu/lb°F

Available sponge volume of matrix = 6.1 ml/ft^2

5. Hydrogen Storage Tank

Volume	= 2.0 ft^3
Overall thermal conductance to surroundings	= 2.0 Btu/hr-°F
Initial pressure	= 20 psia
Initial mass	= 0.014 lb

6. Filter Characteristics

Removal efficiency	= 0.99

7. Hydrogen Flow to Subsystem

Flow rate	= 0.182 lb/hr
Temperature	= 75°F

8. H_2/CO_2 Accumulator

Volume	= 2.0 ft^3
Overall thermal conductance to surroundings	= 2.0 Btu/hr-°F
Initial pressure	= 20 psia
Initial mass of hydrogen	= 0.014 lb
Initial mass of carbon dioxide	= 0.0618 lb

2.5 SOLID ELECTROLYTE

2.5.1 Process Description

Although the solid electrolyte process is conventionally categorized as a CO_2 reduction scheme, and therefore not in the same functional category as the previous CO_2 management concepts, it has some unique features that warrant discussion.

The solid electrolyte process (see References 5.10 and 5.11) in conjunction with a CO disproportionation reactor results in the reduction of CO_2 to carbon and oxygen. A small amount of water vapor in the CO_2 feed, which enhances the main reaction, is simultaneously electrolyzed to hydrogen and oxygen. Reference (5.12) points out that close coupling of this system with a carbon dioxide concentrator which generates humidified carbon dioxide continuously would have operational advantages. All of the previous writeups on the various CO_2 management concepts implicitly assumed that "dry" CO_2 was the desired product, mainly because the Sabatier or Bosch reactions were envisioned as the next step. The reason for discussing the solid electrolyte process, therefore, is to emphasize that humidified CO_2 might be the desired product from a CO_2 concentrator in some trade-off studies.

The system is composed of cells consisting at a solid electrolyte mixture of 91.25 mole percent zirconia (ZrO_2) and 8.75 mole percent yttria (Y_2O_3). This solid electrolyte is situated between two platinum electrodes to which the electrolyzing potential is applied. The basic electrochemical separation process which occurs is illustrated in Figure 2.5-1. For a gas stream including carbon dioxide and water vapor the following reactions occur at the cathode:

$$2CO_2 + 4e^- \longrightarrow 2CO + 2\,O^=$$
$$H_2O + 2e^- \longrightarrow H_2 + O^=$$

At a temperature of 525-700°C (1000-1300°F), the $O^=$ ions will be transported across the oxide film by the influence of the potential gradient. The reactions are enhanced by the presence of H_2O in the gas stream. The oxygen ion then migrates under the influence of a potential field through vacancies in the crystal lattice of the solid electrolyte material to the anode, where the oxygen ion is converted to an oxygen atom. The solid electrolyte is essentially impermeable to non-ionic species (in particular it is impermeable to CO) so that pure O_2 is formed at the anode and may be sent to

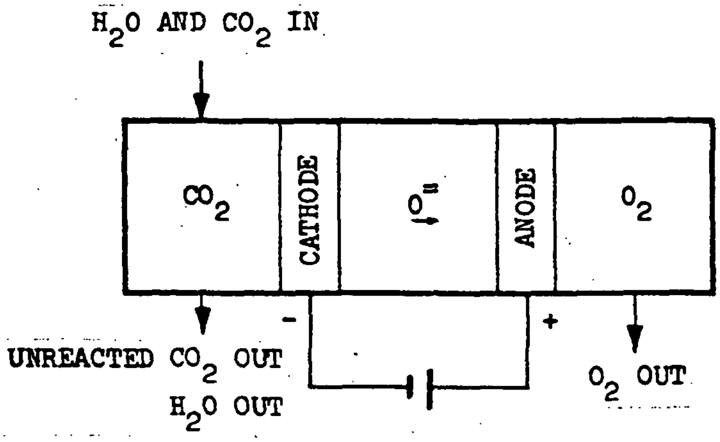


FIGURE 2.5-1 SOLID ELECTROLYTE CELL REACTIONS

the cabin with no further processing other than cooling. The power consumption in the cell is split between energy required to decompose the CO_2 and the resistance heating of the solid electrolyte material. As the predicted cell efficiency is thought to be good and the operating temperature high, this unit must be well insulated to prevent heat leakage which would decrease unit performance. An auxiliary heater in the cell tube is designed to bring the tube to operating temperature.

The free energy change involved in the decomposition of CO_2 to carbon monoxide and to oxygen is 123 kcal/gram-mole of oxygen. This corresponds to a theoretical power requirement for a cell of 68.8 watts/kg of CO_2 per day.

The mixture of CO and CO_2 from the cell cathode is passed through a catalytic reactor which converts CO to CO_2 (returned to the electrolytic cell) and to solid carbon. The free energy change in this reaction is 29 kcal/gram-mole of carbon. This corresponds to a heat dissipation requirement of 45 watts/kg of CO_2 per day.

A flow diagram of a solid electrolyte system is given in Figure 2.5-2 which shows that after leaving the electrolyte cell, a separator is used to remove hydrogen from the gas stream. Also, a regenerative heat exchanger is used to cool the gas products to approximately 950°F, which is the operating temperature of the catalytic reactor. In the catalytic reactor, the carbon monoxide is dissociated to form carbon and carbon dioxide over a nickel or stainless steel catalyst. When the resultant carbon has built up to a high level, a pressure switch will sense the increasing differential pressure and signal for a change of catalyst bed. The catalytic reaction is exothermic and no heating of this unit is necessary once the system has reached operating temperature. A heat exchanger is used to remove the excess heat of reaction from the gas stream. A blower draws the recycle and process gases through the regenerative heat exchanger and humidifier before returning them to the electrolytic reactor.

2.5.2 Simulation of Concept

Two distinct cell designs have been fabricated and successfully tested. The first as reported in Reference 5.1 uses solid electrolyte discs between which the electrical potential is applied. The second which is reported in Reference 5.2 uses solid electrolyte tubes. Here the potential is applied at electrodes located on the inside and outside surfaces of the tubes. The second cell design differs from the first in that it incorporates a semipermeable palladium membrane for separating hydrogen from the exit products.

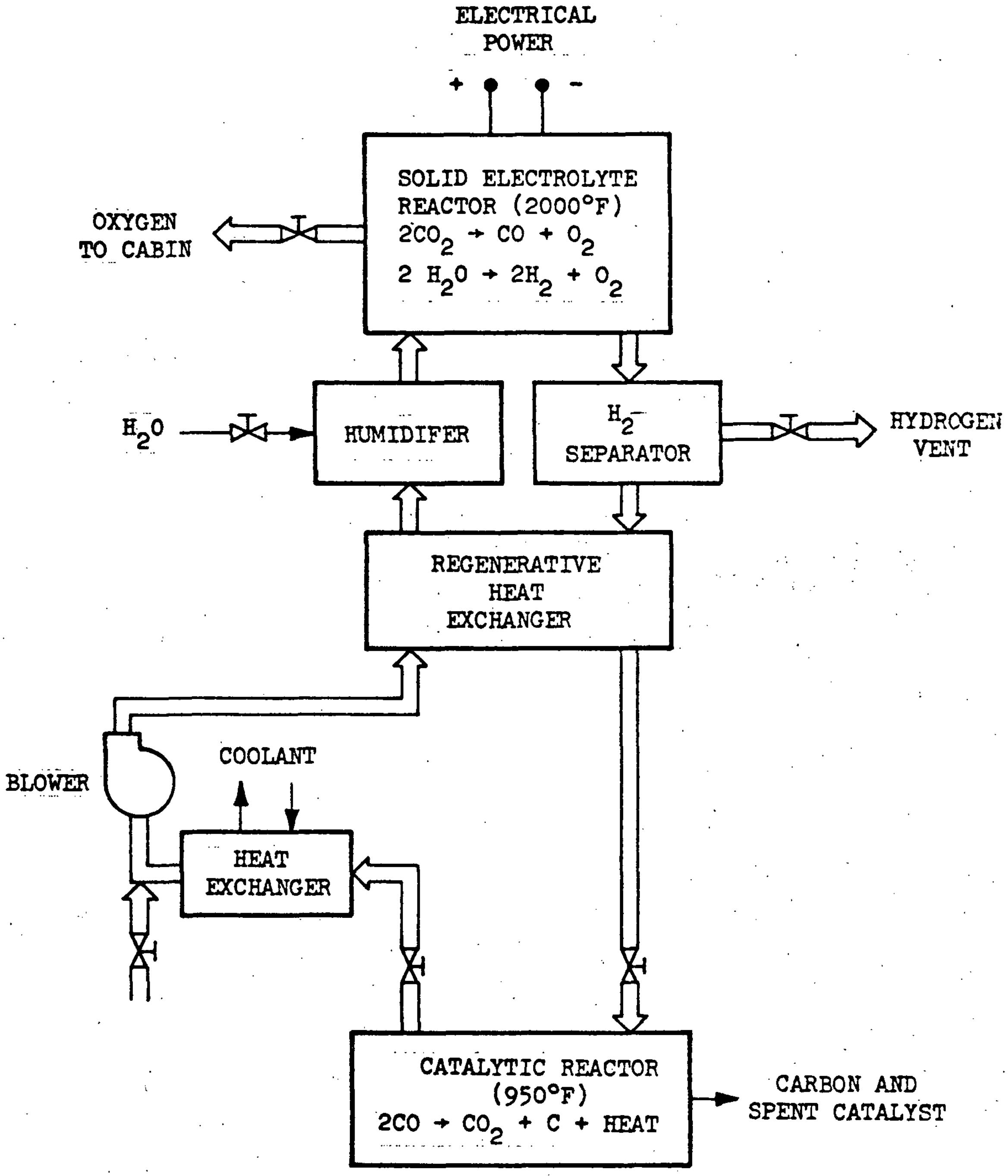


FIGURE 2.5-2 SOLID ELECTROLYTE SCHEMATIC

Relatively low concentrations of hydrogen in the inlet to the reactor have been found to increase the rate of carbon formation. Higher concentrations will shift the chemical equilibrium away from carbon formation. The semi-permeable membrane provides a means for regulating the concentration of hydrogen and thus carbon formation.

Figure 2.5-3 illustrates the G-189A components required to simulate the system for the 180 day life test reported in reference 5.2

CO_2 flow to the subsystem is supplied from CO_2 accumulator component 1 (TANKG). The CO_2 stored in this tank is assumed to have been collected by a CO_2 concentration subsystem. The steam desorbed solid amines, hydrogen depolarized cell, or carbonation cell concepts are then potentially suitable for this purpose. CO_2 flow is moved by component 2(FAN) to humidifier component 3 (GASMIX). Here the CO_2 is saturated with water prior to entering the solid electrolyte cells. The saturated CO_2 joins with recycle flow at component 4 (GASMIX) and then passes into the solid electrolyte cell component 5 (SØLELC).

Component 5 represents several parallel modules of solid electrolyte cells. Each module is composed of a number of parallel stacks of electrolysis cells. CO_2 is electrolytically decomposed into O_2 and CO in the cells. Water also is electrolyzed into hydrogen and oxygen. Oxygen collected at the anode of the cells flows to oxygen accumulator tank component 6 (TANKG).

CO and H_2 products and unreacted CO_2 and H_2O reactants flow to hydrogen gas separator component 7 (MEMOD). Hydrogen is separated by selective diffusion through a semi-permeable membrane. Hydrogen separated in this component is moved by vacuum pump component 9 (VACPMP) to hydrogen accumulator component 9 (TANKG).

The primary side gas stream from the hydrogen separator flows to carbon deposition reactor component 10 (CARDP). Here CO is reconverted back into CO_2 for cycling to the solid electrolyte cells. In a secondary reaction,

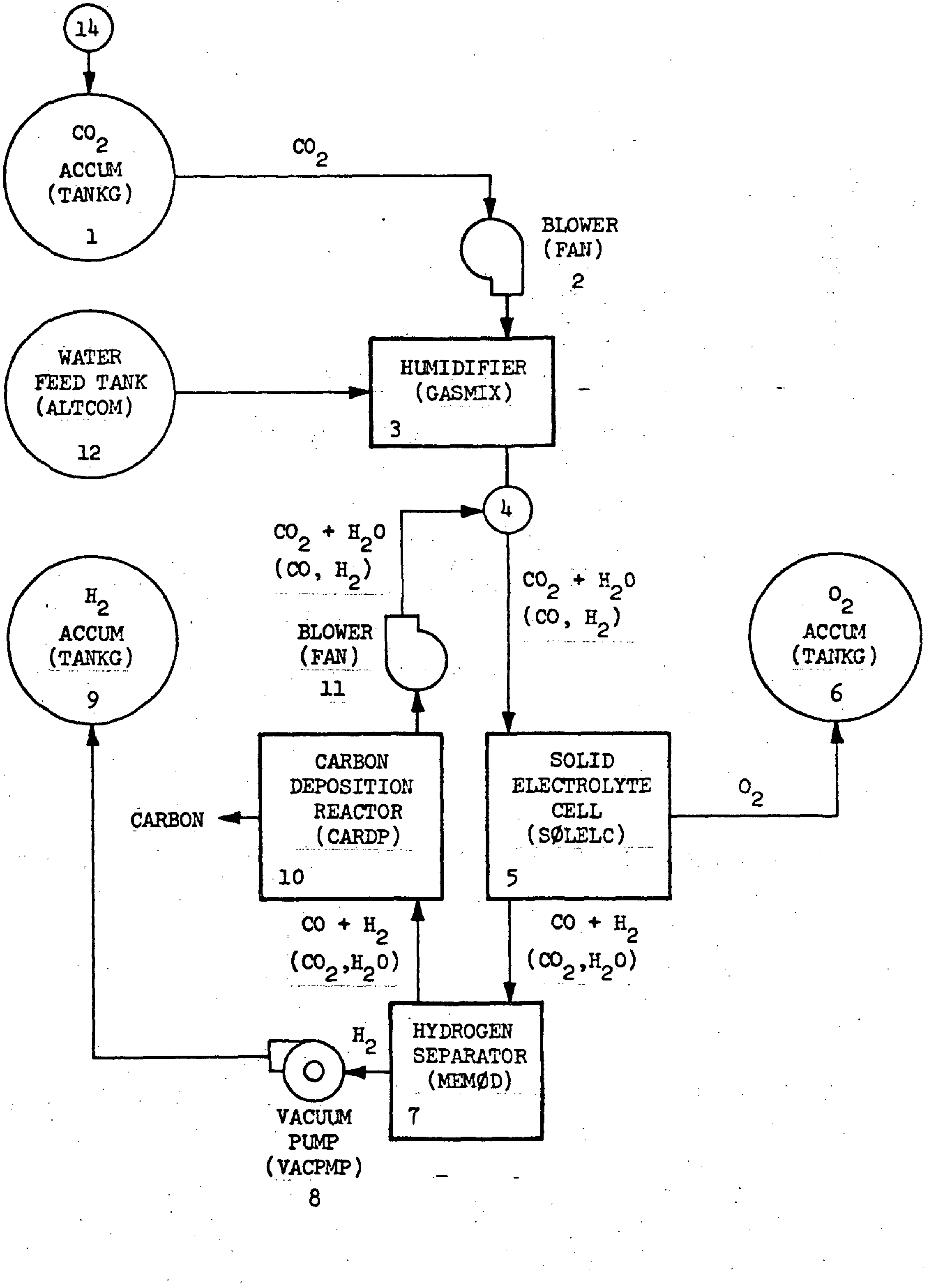


FIGURE 2.5-3 G189A SIMULATION OF SOLID ELECTROLYTE SUBSYSTEM

H_2 reacts with CO_2 to form H_2O and CO. The effluent of this component is circulated by component 11 (FAN) back to combine with the subsystem CO_2 feed gas.

2.5.3 Sample Problem

<u>Description</u> -

A sample problem was prepared for the subsystem illustrated in Figure 2.5.3. The unit is sized for a six-man subsystem. Data has been scaled up from data presented in reference 5.2 and 5.13.

<u>Assumptions</u> -

1. CO_2 from Concentrator Unit

Flow

CO_2	0.542 lb/hr
Water vapor	0.00001
O_2	0.00001
N_2	0.00001
Trace contaminants	0.00001
H_2	0.00001
CO	0.00001

Pressure

Total pressure	14.22 psia

2. Blower characteristics

Heat dissipated into process gas	2.0 watts

3. Humidifier

Water vapor flow rate	0.1230 lb/hr

4. Solid Electrolyte Unit

Number of modules	8
Number of stacks/module	18
Number of cells/stack	7
Temperature = 1652°F	
Thermal conductance between surface of module insulator and ambient gas	2.1 Btu/hr-°F
Thermal conductance of insulation	.222 Btu/hr-°F
Heat dissipated by electrical heater	505. Btu/hr
Total current to unit	135 amps
Overall current efficiency	.810 fraction
CO current efficiency	.825 fraction
H_2 current efficiency	.175
Cell voltage (1.74 - 1.85)	1.8 volts
Voltage efficiency	0.614 fraction
Module thermal capacitance	4. Btu/°F
Active area/cell	6 cm^2
Degree of decomposition	0.55 - 0.6
Current density	160 ma/cm^2

5. Hydrogen Separator

Total membrane area	1.48 ft^2
Thickness of membrane	.005 inches
Permeability	$5.18 \times 10^{-4} \ \frac{\underline{ft^3/hr\ (inches)}}{ft^2\ (mm\ Hg)}$
UA to surroundings	.1 Btu/hr-°F
UA across membrane	100. Btu/hr-°F
Number of membranes	1
Frontal area (primary side)	0.2 ft^2
Frontal area (secondary side)	0.01 ft^2
Cell length	0.662 ft
Module thermal capacitance	0.1 Btu/°F
UA cell to module	1.0 Btu/°F

6. Carbon Deposition Reactor

CO conversion	.212 (fraction)
H_2 conversion	0. (fraction)
Heat dissipated by electrical heater	1000. (Btu/hr)
Reactor thermal capacitance	2. (Btu/°F)
Operating temperature	986 (°F)

7. Recycle Blower

Heat dissipated into process gas	60 watts

8. O_2 Accumulator

Volume	2.0 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr-°F
Initial pressure	14.7 psia
O_2 use rate	0.5 lb/hr
Initial mass fraction O_2	1.0 fraction

9. Vacuum Pump Characteristics

Isentropic compression

η_{areo}	0.40
η_{motor}	0.60
K = polytropic exponent	1.41 (H_2 @ 15°C)

Flow determined from generalized curve for small vacuum pumps (See Figure 2.2-3)

10. Hydrogen Accumulator

Volume	2.0 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr-°F
Initial pressure	14.7 psia
Initial mass in tank	.3 lb

11. CO_2 accumulator

Volume	2.0 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr-°F
Initial pressure	14.7 psia
Initial mass in tank	.3 lb

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
   a. Number of cells per stack
   b. Number of stacks per module
   c. Number of modules per unit
   d. Cell current
   e. Cell electrode area

2. When attempting to match predicted results with experimental results for the same cell configuration, the following parameters should be varified:
   a. Overall O_2, CO, and H_2 current efficiency
   b. Power efficiency
   c. Cell voltage and current
   d. Cell dimensions
   e. Heat transfer characteristics
   f. Reactor conversion

2.6 Liquid Absorption

2.6.1 Process Description

This process uses a liquid solution of potassium or sodium carbonate, or a mixture of both, to absorb CO_2 from the cabin air. When carbon dioxide is absorbed in an aqueous solution of sodium or potassium carbonate, the following reversible reaction occurs:

$$K_2CO_3 + CO_2 + H_2O \rightleftarrows 2KHCO_3$$

Heating the bicarbonate solution and reducing the partial pressure of carbon dioxide in the gas stream causes bicarbonate to be reconverted to carbonate and CO_2.

The amount of carbon dioxide absorbed depends on several factors. These include the fraction of base that is bicarbonate, the normality of the solution, and the partial pressure of carbon dioxide in the gas. The relationship between these variables at equilibrium conditions is given by the following equation (Reference 6.19).

for $K_2CO_3/KHCO_3$

$$P_{CO_2} = \frac{45 f_o^2 N^{1.29}}{S(1-f_o)(302-t)}$$

for $Na_2CO_3/NaHCO_3$

$$P_{CO_2} = \frac{137 f_o^2 N^{1.29}}{S(1-f_o)(365-t)}$$

where:

P_{CO_2} = partial pressure of CO_2 (mmHg)

N = normality of base $\left(\frac{\text{g equivalents}}{\text{liter}}\right)$

S = solubility of CO_2 in H_2O at one atmosphere $\left(\frac{\text{g moles } CO_2}{\text{liter } H_2O}\right)$

t = temperature (°F)

f_o = fraction of total base that is bicarbonate

A schematic of a CO_2 concentrator subsystem using the liquid absorption concept is shown in Figure 2.6-1. CO_2 laden cabin air is introduced into a contactor where the air stream is mixed with an aqueous carbonate solution to promote absorption of CO_2. The absorption reaction is favored when the solution is approximately at room temperature. In industrial gas/liquid absorption processes, counter current flow is commonly used. However, it is difficult to envision a counter flow contactor for zero-g operation. Since a suitable zero-g design has not been yet defined, the contactor has been assumed to operate with co-current or parallel flow. A device for gas/liquid separation is located immediately downstream of the contactor to achieve separation of the cabin air stream from the carbonate solution.

A regenerative heat exchanger and external heat source is used to heat the carbonate solution prior to entering a liquid flash vaporizer. Here, CO_2 is desorbed and a portion of the water in the solution is vaporized. The liquid and gas phases leaving the vaporizer are assumed to be in thermodynamic and chemical equilibrium. The liquid phase is recirculated back to the liquid contactor and the gas phase is pumped to a condenser/separator where CO_2 is separated from water vapor. The CO_2 is then transferred to a CO_2 storage tank.

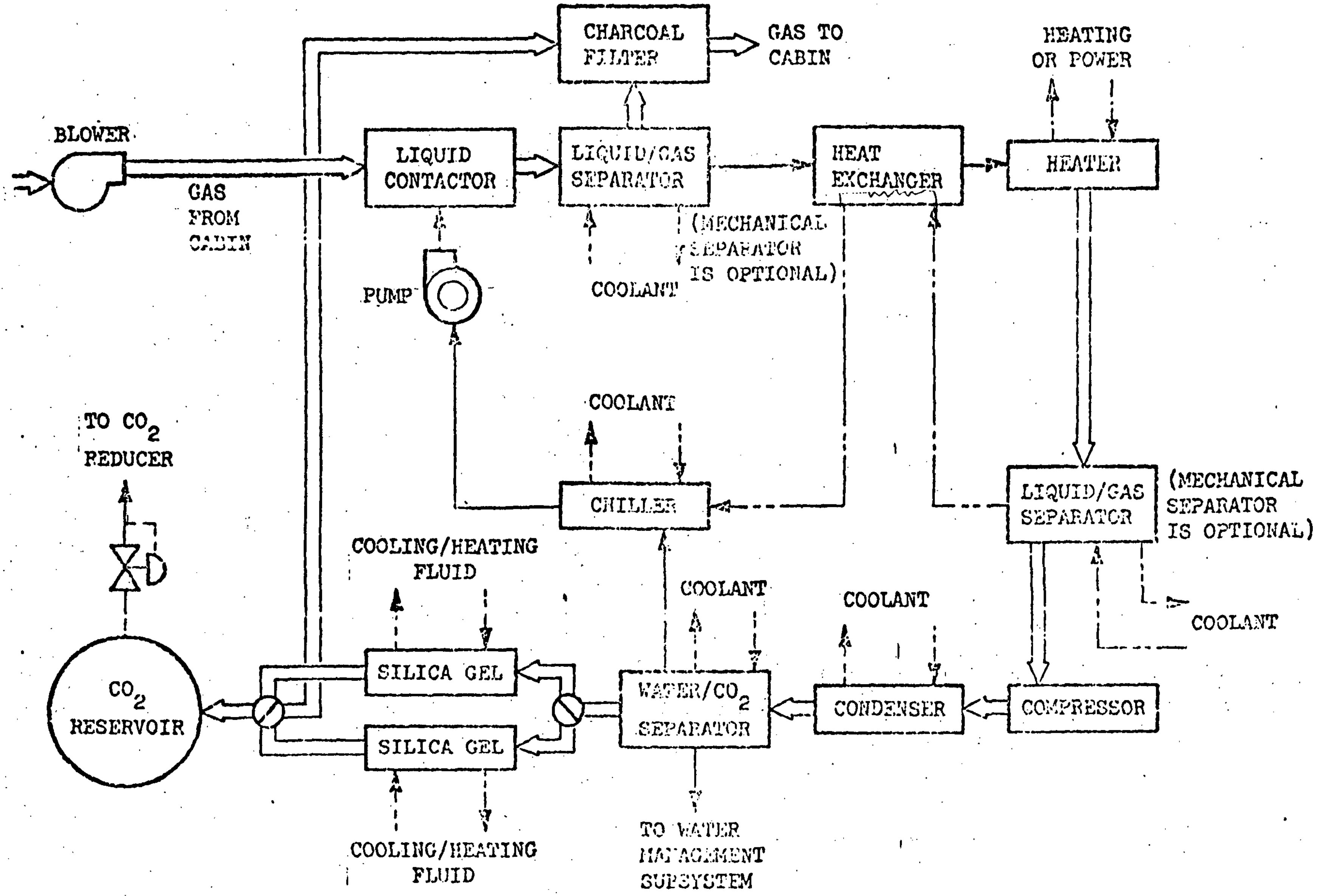


FIGURE 2.6-1 LIQUID ABSORPTION CO_2 CONCENTRATOR

2.6.2 Simulation of Concept

A simulation model of the liquid absorption CO_2 concentrator subsystem was prepared to facilitate evaluation of the concept and to define the subsystem's critical components and parameters such as solution flow, temperature, and pressures. Figure 2.6-2 shows the G-189A components required for a typical subsystem. Inlet air, defined by component 1 (ALTCØM) is forced into the liquid contactor by blower component 2 simulated by subroutine FAN. The liquid contactor, component 3, is simulated by subroutine LIQCØN. This subroutine determines the amount of CO_2 absorbed in a parallel flow contactor with the gas and liquid phases leaving in thermal and chemical equilibrium. The effluent from the contactor flows to component 4 (SPLIT) where the CO_2 free cabin air is separated from the carbonate/bicarbonate solution. The air stream is dehumidified in component 5 (ANYHX) prior to being returned to the cabin.

The carbonate/bicarbonate solution flows through regenerative heat exchanger component 7 (ANYHX) and heater component 8 (ALTCØM) to raise the solution temperature to approximately 180°F. The solution then is partially vaporized in flash evaporator component 9 (LQFLSH). CO_2 is desorbed into the gas phase as a result of the partial vaporization. The gas phase which evolves contains CO_2 plus H_2O vapor. The liquid phase, which is in equilibrium with the gas phase, is a mixture of H_2O, carbonate, and bicarbonate.

The gas phase generated in the flash vaporizer is separated from the liquid phase and pumped by compressor component 16 (FAN) to condensing heat exchanger component 10 (ANYHX). Here, H_2O vapor is separated from the CO_2. The CO_2 then flows to CO_2 reservoir component 12 (TANKG). The liquid phase from the flash vaporizer (component 9) is recirculated by pump component 19 (PUMP) back through the regenerative heat exchanger (component 7). The solution then is chilled in heat exchanger component 15 (ANYHX) prior to returning to the liquid contactor (component 3).

Water vapor condensed and separated in components 5 and 10 is collected by component 13 (H20SUM) and transferred to storage tank component 14 (TANKG). Makeup water to the carbonate/bicarbonate loop is supplied by this component. This water enters the loop at component 17 (LIQMIX).

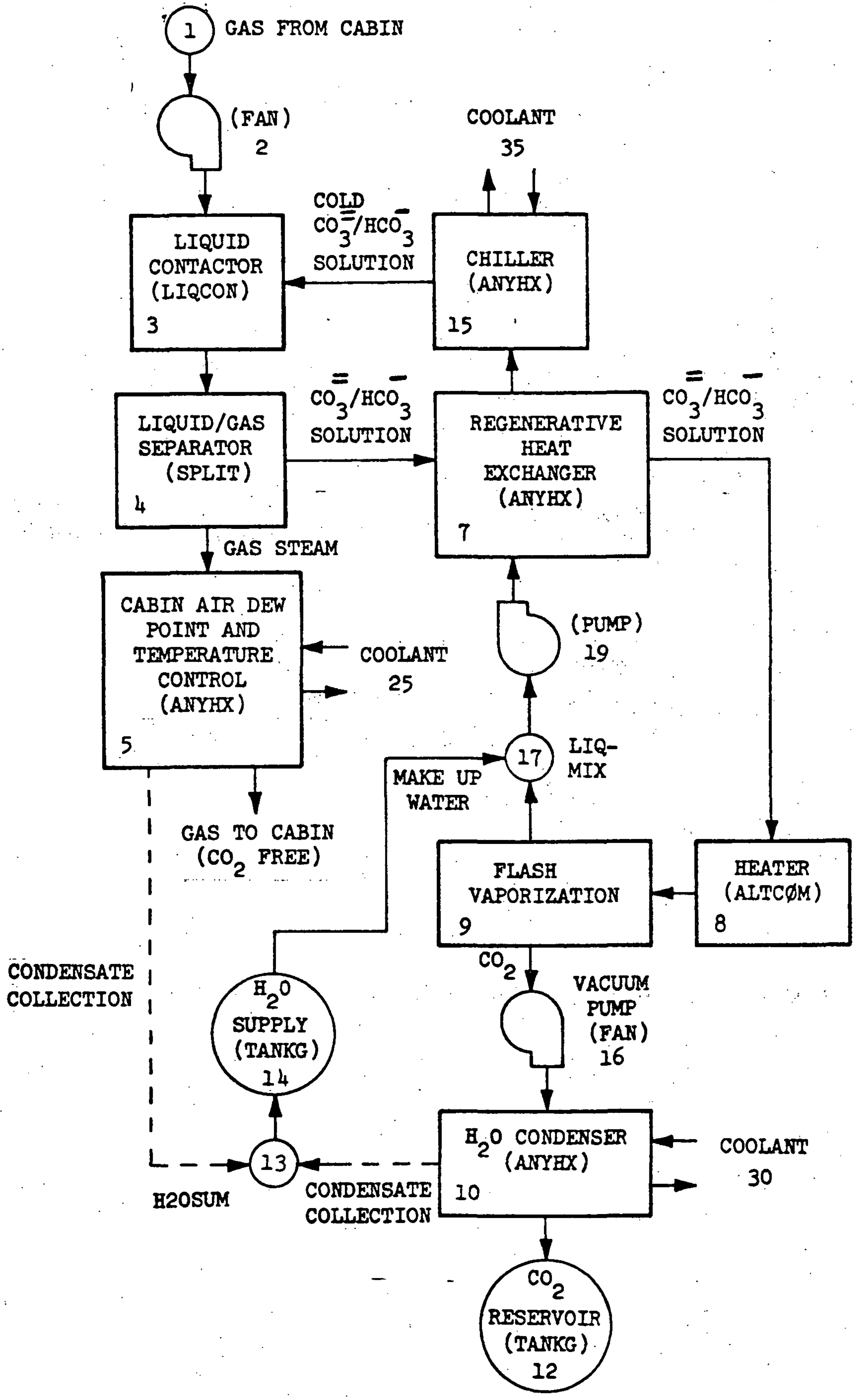


FIGURE 2.6-2 G-189A SIMULATION OF LIQUID ABSORPTION CO_2 CONCENTRATOR

2.6.3 Sample Problem

Description -

A sample problem simulating major components of the liquid absorption CO_2 concentrator subsystem has been prepared for performance analysis and system evaluation. The inlet conditions of the sample problem, shown schematically in Figure 2.6-2, are defined by a dummy component simulating cabin air flow to the system. The data defined by the dummy component include total flow, cabin air temperature and pressure, noncondensable flow, condensable vapor flow, specific heat and molecular weight of the noncondensable flow, oxygen flow, diluent flow (N_2), and CO_2 flow. The input values to the first component are derived from assumptions defining cabin air conditions and the CO_2 removal rate and efficiency of the subsystem. The inlet conditions and flow rates along with the performance characteristics of the subsystem were used in the derivation of the design parameters of individual components.

Assumptions -

1. The cabin air conditions and system requirements are as follows:

Dry bulb temperature, °F	70.
Wet bulb temperature, °F	60.
Cabin pressure, psi	14.7
Partial pressure CO_2, mmHg	3.0
O_2 pressure, psi	3.1
CO_2 generation/removal rate per man $\frac{\text{lb}}{\text{hr-man}}$	.1
Number of men	6

The total cabin air flow into the system is dependent on the required CO_2 removal rate, the concentration of CO_2 in the cabin air, and the CO_2 removal efficiency of the liquid absorption subsystem. The CO_2 removal rate and concentration in the cabin air are fixed by the rules used in evaluating the various CO_2 concentrator subsystems. The CO_2 removal efficiency is dependent on the temperature of the aqueous solution flowing into the liquid contactor and the fraction of base that is bicarbonate. Lower bicarbonate fraction results in much higher sybsystem efficiency and, reducing the amount of carbonate solution that is required in CO_2 absorption and the amount of cabin air that is required to be passed through the system. Using the value of .23 for the CO_2 removal efficiency of the liquid contactor, we determine the required volumetric flow through the system to equal 4980 ft^3/hr from which derive the input values to component 1.

Total flow, lb/hr	368.283
Temperature, °F	70.
Pressure, upstream duct, psi	14.7
Pressure, component outlet, psi	14.7
Noncondensable flow, lb/hr	364.201
Condensable vapor flow, lb/hr	4.082
Noncondensable specific heat, Btu/lb-°F	.24
Noncondensable molecular weight	28.97
Oxygen flow, lb/hr	96.92
Diluent flow (N_2), lb/hr	265.08
CO_2 flow, lb/hr	2.201

2. The blower forcing air into the system is simulated by subroutine FAN only to an extent that heat is added to the flowing gas stream. The value for heat added to gas stream by the blower is 50 watts.

3. Liquid Contactor characteristics (CO_2 absorption)
   The CO_2 absorption, and thereby removal from the cabin air stream, is accomplished by component 3, liquid contactor.

   The component is simulated by the new subroutine LIQCON with the required input being as follows:

CO_2 removal efficiency of the contactor	.23
Fraction of base that is bicarbonate in solution entering contactor (mole fraction)	.37
Normality of the solution entering the contactor	1.0

The inlet flow rates of constituents of the aqueous carbonate solution required to meet the CO_2 removal requirements and the system characteristics are computed on the first system pass when the value of Instruction Option 2 is set to 1. Instruction Option 1 selects type of solution, sodium carbonate/potassium carbonate, that is being used. The sample run assumed that the solution used is potassium carbonate.

4. Liquid/Gas Separation

The separation of the liquid and gas is accomplished by component 4, simulated by subroutine SPLIT. The input data required is as follows:

SPLIT ratios for flows A(6), A(7), A(10), A(11), and A(12)	0.
SPLIT ratios for flows A(15), A(16), A(17)	1.

5. Heat Exchanger Characteristics (cabin air temperature and humidity control)

The gas stream flowing through the liquid contactor where it is mixed with aqueous solution becomes saturated with vapor. Component 5, simulated by subroutine ANYHX, is used for condensing the cabin air temperature to 60°F dew point temperature. The only input requirement is the overall UA (Btu/hr-°F) of the heat exchanger which is set equal to 130.

The secondary flow is provided by component 25 with inlet conditions defined by the following:

Flow rate, lb/hr	150.
Temperature, °F	45.
Pressure, psi	15.

The physical properties of the coolant (water), are listed as follows:

Specific heat, Btu/lb-°F	1.0
Viscosity, lb/hr-ft	3.6
Density, lb/ft^3	62.4
Molecular weight, lb/mole	18.0
Conductivity	.325

is the desired normality of the aqueous solution, set to 1.0. It is used in determining the amount of makeup water that is required to account for vaporization.

The heat loss to surrounding data is as follows:

Ambient gas temperature, °F	70.
Thermal conductance between surface and ambient, Btu/hr-°F	.5
Ambient wall temperature, °F	60.
FA factor for radiation conductance, ft^2	8.0
Structure temperature, °F	60.
Conductance between module and structure	.1
Conductance between module surface and insulation	.3

10. The gas from the liquid flash vaporization module is removed by component 16 which is simulated by subroutine FAN. The component is simulated only to an extent that heat is added to the gas stream flowing through. The required input is heat added to gas stream, 10 watts.

11. H_2O/CO_2 Condensing Heat Exchanger Characteristics

The separation of H_2O/CO_2 is accomplished by component 10, simulated by subroutine ANYHX. The required input defining the heat exchanger is the overall thermal conductivity, UA= 100. The secondary flow, water, provided by component 30 is defined as follows:

Flow rate, lb/hr	250.
Temperature, °F	45.
Pressure, psi	10.

12. CO_2 Accumulator Tank

Storage of CO_2 gas is accomplished by component 12, simulated by subroutine TANKG. The required inputs are as follows:

The physical properties listed above also apply to coolant flow from components 30 and 35, which provide secondary flow to components 10 and 15, respectively.

6. Flow Return to Cabin

The return of CO_2 depleted cabin gas stream is simulated by subroutine FLOMET. The only input required is the reference temperature for enthalpy which is set at 32°F.

7. Regenerative Heat Exchanger Characteristics

The efficiency of the regenerative heat exchanger determines the power requirements for the system. A heat exchanger of high efficiency results in lower power requirements and a smaller heat exchanger to be used in chilling the aqueous solution. The regenerative heat exchanger is simulated by subroutine ANYHX as component 7. The required input is the parameter defining the size of the heat exchanger, overall thermal conductivity UA. The value of UA, Btu/hr-°F, is 1385.

8. Component 8, simulated by subroutine ALTCOM, heats the aqueous solution to desired temperature prior to lowing it into the liquid flash vaporizer. The input required is the desired outlet temperature, which is set to 185°F.

9. Liquid Flash Vaporization Module Characteristics

The desorption of CO_2 from the aqueous carbonate solution is accomplished by component 9, simulated by subroutine LQFLSH. Probably the most critical input parameter of the component and the subsystem is the nominal CO_2 partial pressure in the exit gas flash vaporization module, set initially to 10 mmHg in this sample run. This parameter determines the percentage of bicarbonate that will decompose evolving CO_2 gas and the fraction of base that is bicarbonate leaving the flash vaporization module. As mentioned in section 3.0, the CO_2 removal efficiency of the liquid contactor is heavily dependent on the fraction of base that is bicarbonate flowing into the contactor, the lower fraction resulting in higher efficiency. The other required input parameter

Ambient Gas Temperature, °F	70.
Thermal Conductance Between Ambient Tank, Btu/hr-°F	5.
Ambient Wall Temperature, °F	60.
Radiation FA Skin to Wall, ft^2	6.
Structure Temperature, °F	60.
Conductance between Tank and Structure, Btu/hr-°F	12.
Total Fluid Weight in Tank, lb	0.5
Fluid Temperature in Tank, °F	70.
Fluid Volume in Tank, ft^3	1.
Fluid Press in Tank, psi	14.7
Weight of Noncondensable in Tank, lbs	0.5
Noncondensable Specific Heat in Tank, Btu/lb-°F	.17
Noncondensable Molecular Weight, lb/mole	44.
Weight of CO$_2$ in Tank, lb	0.5

13. The collection of water condensate, condensing in components 5 and 10, is accomplished by component 13 simulated by H20SUM. The required inputs are as follows:

Number of components providing condensate	3.
Component number of first component providing the condensate	5
Component number of the second component providing the condensate	10

14. Water Storage Tank Characteristics

Water supply tank (component 14) which may be used to provide makeup water to the liquid absorption subsystem or to store excess water that might be condensed is simulated by subroutine TANKG. The required inputs are as follows:

Ambient Gas Temperature, °F	70.
Conductance Surface Insulation to Ambient, Btu/hr-°F	5.
Ambient Wall Temperature, °F	60.
Radiation FA Factor, ft^2	6.
Structure Temperature, °F	60.
Conductance between Wall and Insulation, Btu/hr-°F	.05
Total Fluid Weight in Tank, lb	62.4
Fluid Temperature in Tank, °F	60.
Fluid Volume in Tank, ft^3	1.
Weight of Liquid, lb	62.4
Maximum Allowable Temperature Change for SS, °F	5.0

15. Component 7, simulated by subroutine LIQMIX, provides a method of adding water from the storage tank to the liquid absorption subsystem. There are no inputs required.

16. The aqueous solution is circulated through the system by component 18 simulated by subroutine PUMP. The pump is simulated only to an extent that heat is added to the system. The value of heat added to the system is assumed to be 100 watts.

17. Chiller Characteristics

The chiller (component 15) used in reducing the temperature of aqueous carbonate solution is simulated by subroutine ANYHX. The required input defining the size of the chiller is its overall thermal conductivity UA (Btu/hr-°F)=600.

The secondary flow defined by component 35 is as follows:

Flow rate, lb/hr	100.
Temperature, °F	45.
Pressure, psi	10.

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
   a. Flash evaporator pressure and temperature
   b. Process gas and carbonate solution flow rate

2. When attempting to match predicted results with experimental results for the same cell configuration, the following parameters should be varified:
   a. CO_2 equilibrium data
   b. Heat transfer characteristics

2.7 ELECTRODIALYSIS

2.7.1 Process Description:

A sketch of a typical Electrodialysis CO_2 Management System is given in Figure 2.7-1. The most important components are the electrodialysis stacks since it is here that carbon dioxide is removed from air and oxygen is generated from water simultaneously. In general, cabin air is humidified and fed to absorber compartments where the carbon dioxide in the air is electrochemically converted to carbonate ions. Under the influence of an electrical potential, the carbonate ions are transferred out of the absorber into concentrator compartments where they react further to reform carbon dioxide gas. At the electrodes (anodes and cathodes) water is electrolyzed to form oxygen and hydrogen. Thus, if the system were treated as a black box, there are two inlet streams: water and cabin air containing carbon dioxide, and four effluent streams: oxygen, hydrogen, air with a reduced carbon dioxide content, and carbon dioxide (of greater than 99% purity). The basic principles involved in the electrochemical operations are electrodialysis and electrolysis. The description which follows was abstracted from Reference 7.2.

Electrodialysis is a process in which ionized molecules or atoms are transferred through highly selective ion-transfer membranes under the influence of a direct current. If a solution containing positively and negatively charged ions is fed to an electrodialysis cell, the positively charged ions (cations) will be attracted to the positively charged anode. The nature of the ion-transfer membrane between the solution and electrode (anode or cathode) determines whether or not an ion can migrate through it or be retained in the solution.

Anion-transfer membranes will allow anions to pass through them but exclude cations, while cation transfer membranes will allow the passage of cations but not anions. These membranes are highly selective for either anion or cation transfer. It is the selective properties of the anion and cation membranes which allow CO_2 to be removed from the process air in one compartment while CO_2 is concentrated in an adjacent compartment. The two adjacent compartments are termed a cell pair. It is possible in this sort of arrangement to place as many as 500 cell pairs between a single pair of electrodes. The combination of cell pairs and electrodes is referred to as an electrodialysis stack.

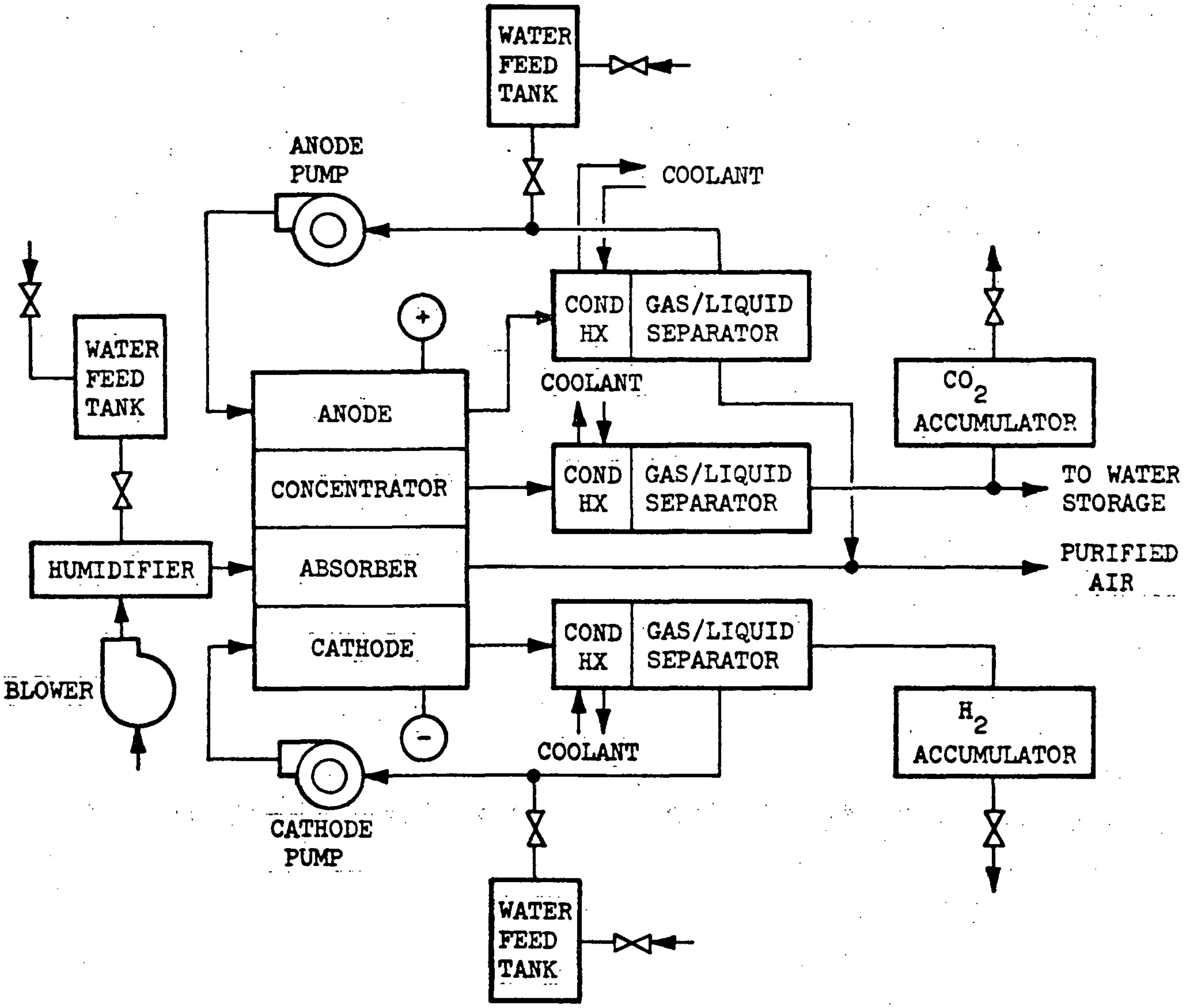


FIGURE 2.7-1 ELECTRODIALYSIS CO_2 MANAGEMENT SYSTEM

The CO_2 removal unit is comprised of repeating units consisting of four compartments: a carbon dioxide absorber, or scrubber; a concentrator compartment; an anode; and a cathode. The absorber and concentrator compartments can be termed a cell pair, while the anode and cathode compartments represent an electrode pair. The reactions which occur in the various compartments of this configuration are summarized in Figure 2.7-2.

The operation of the CO_2 removal unit is as follows:

Liquid (demineralized water is fed to the cathode compartment at a rate at least sufficient to provide for the water lost by electrolysis at the cathode,

$$H_2O + e^- = \frac{1}{2}H_2 + OH^-$$

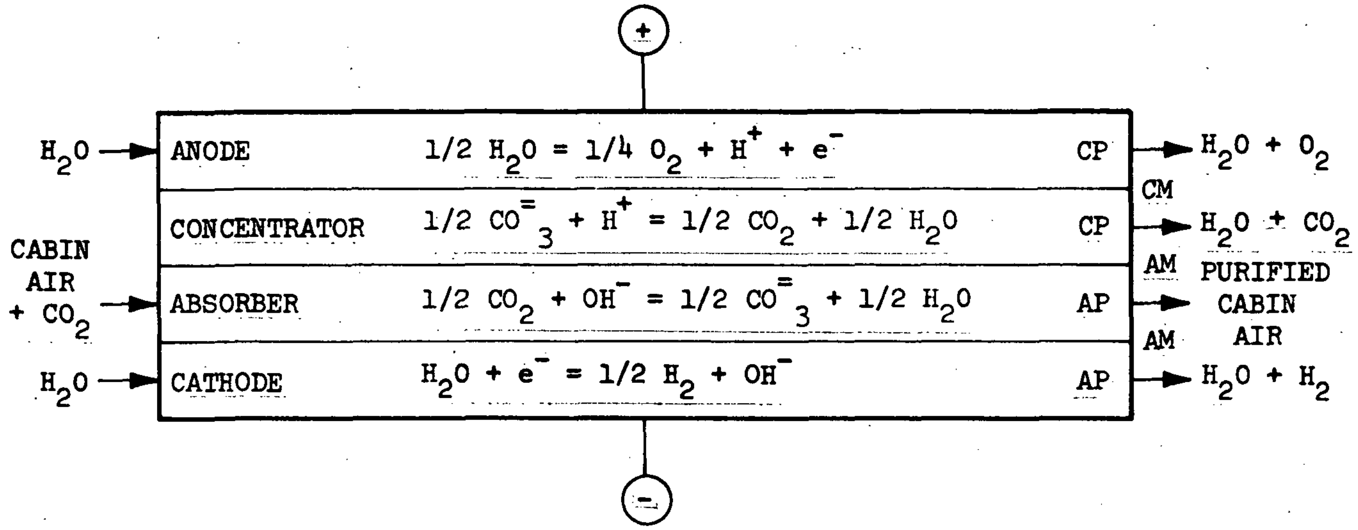
and by electroendosmosis through the anion membrane into the absorber compartment. In any electrodialysis process as ions migrate across the membranes, water is transferred in the same direction. This water is apparently transferred due to the hydration of the ions as well as the electrical potential created by the movement of the ions through the pores of the membranes. The total water transfer is referred to as endosmotic water.

The liquid flow rate will be in excess of the electrochemical requirements to provide cooling of the stack and a sweep stream for the evolved hydrogen gas. A flow rate of about 8 gallons per hour is recommended in Reference 7.2 for a six-man unit at a cabin pressure of 7 psia.

Cabin air containing carbon dioxide is humidified and fed to the absorber compartment. In this compartment, which contains anion-exchange materials in the OH^- form, carbon dioxide is scrubbed from the air according to the following reaction,

$$\frac{1}{2}CO_2 + OH^- = \frac{1}{2}CO_3^{=} + \frac{1}{2}H_2O$$

The anion-exchange material is continually regenerated by the migration of hydroxyl ions from the cathode into the absorber compartment.



CM = CATION PERMSELECTIVE MEMBRANE
AM = ANION PERMSELECTIVE MEMBRANE
CP = MACROPOROUS CATION PERMSELECTIVE PACKING
AP = MACROPOROUS ANION PERMSELECTIVE PACKING

FIGURE 2.7-2 CO_2 REMOVAL UNIT (BASIC REPEATING UNIT SHOWN)

Carbonate ions, excess hydroxyl ions and endosmotic water are transferred from the absorber into the concentrator compartment which contains cation-exchange material in the H^+ form. The following reactions occur:

$$\frac{1}{2}CO_3^{=} + H^+ = \frac{1}{2}CO_2 + \frac{1}{2}H_2O$$

$$OH^- + H^+ = H_2O$$

The reformed carbon dioxide gas, along with the endosmotic water, passes out of the compartment under its own pressure.

Liquid (demineralized) water is fed to the anode compartment at a rate at least sufficient to provide for the water lost by electrolysis at the anode,

$$\frac{1}{2}H_2O = \frac{1}{4}O_2 + H^+ + e^-$$

and by endosmosis through the cation membrane into the concentrator compartment. The water flow rate will be substantially in excess of the electrochemical requirements to aid in heat removal from the anode and to provide a sweep stream for the evolved oxygen gas. The hydrogen ions continually migrate into the concentrator compartment, where they serve to regenerate the cation-exchange material.

There is at least some liquid water present in all four streams effluent from the concentrator. This leads to a gravity-independent gas-liquid separation requirement which is readily provided (since no frothing or foaming has been observed) by small state-of-the-art, passive, gas-liquid separators having short holdup times.

The theoretical reactions shown in Figure 2.7-2 assume 100% carbonate ion transfer efficiency and electrode efficiencies. If 100% efficiencies are achieved in all operations in this type of stack, CO_2 is absorbed in a 2:1 volumetric (or mole) ratio to O_2 production. The electrode reactions operate with about 100% efficiencies, while the membrane transfer process actually has efficiencies greater than 100% (under expected operating conditions).

This is explained by the formation of some monovalent bicarbonate ion (HCO_3^-) in the absorber, which (for the same current flow) would transfer twice as much carbon dioxide as the divalent carbonate ion ($CO_3^=$). Thus, the actual volumetric ratio of CO_2 absorption to O_2 production is greater than 2:1.

On the average a man expires 0.85 moles of carbon dioxide for every mole of oxygen inhaled (or a CO_2/O_2 ratio of 0.85:1). If a membrane transfer efficiency of 120% is assumed for normal concentrator operation, then a CO_2/O_2 ratio of 2.4:1 is attained. This means that this type of electrodialysis stack does not supply sufficient metabolic oxygen while removing all the metabolic carbon dioxide. The remaining oxygen must be supplied by some other oxygen generation equipment.

It should be mentioned that experimental work has been conducted on electrodialysis stacks containing only one anode and cathode compartment for a multiple number of absorber/concentrator cell pairs. An additional compartment or water cell is added to each absorber/concentrator cell pair to provide the ncessary H^+ and $\overline{OH}$. By eliminating the anode/cathode compartments with each cell pair, carbon dioxide can be removed from the atmosphere with almost negligible amounts of oxygen generated. However, the power requirements of these stacks have not been much lower than the power requirements of the Carbon Dioxide Scrubber described previously. In addition, between the cabin atmosphere leak rate and the metabolic loss of available oxygen (respiratory quotient of 0.85), there will be a significant oxygen supply requirement no matter what oxygen recovery subsystem is included in the space vehicle design.

2.7.2 Simulation of Concept

Figure 2.7-3 shows the G-189A components required to simulate a typical CO_2 electrodialysis subsystem.

Cabin air is circulated through the concentrator by blower component 10 (FAN). The flow then passes through humidifier component 11 (GASMIX) prior to entering the electrodialysis cell module. Regulation of the humidity level in the process gas is necessary to prevent drying out of cell membranes.

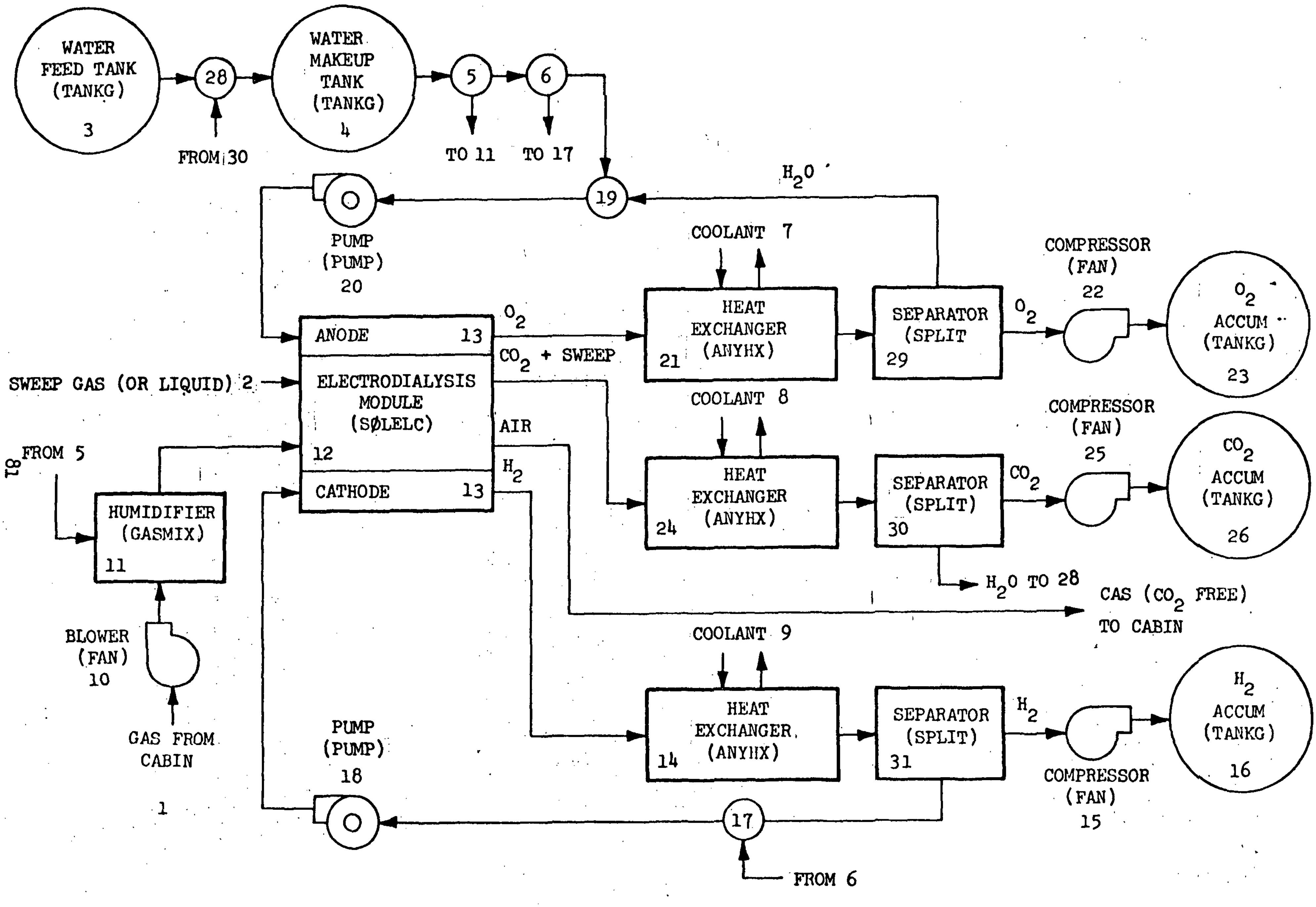


FIGURE 2.7-3 G189A SIMULATION OF ELECTRODIALYSIS CONCENTRATOR

Process gas flows into the absorption compartment of the electrodialysis cell component 12 (ELDIAL). Here, CO_2 is removed by absorption and reaction with $\overline{OH}$ ions. The purified process gas then returns to the cabin or the humidity control subsystem (not shown). The CO_2 removed in the absorption compartment migrates under influence of the cells' electrical field to the concentrator compartment. Here, CO_2 is recovered in a "sweep fluid" provided by component 2. For this sample problem, water is assumed to be the "sweep fluid". The CO_2 picked up by the sweep fluid is separated out in heat exchanger/water separator components 24 and 30 (ANYHX). The CO_2 is compressed by 25(FAN) and transferred to accumulator component 26 (TANKG).

The $\overline{OH}$ and H^+ ions required for the chemical reactions occurring in the absorption and concentrator compartments, respectively, are supplied by water electrolysis reactions in the anode and cathode compartments. An alternate component, 13, is required for storing the outlet flow data for the anode and cathode compartments. Liquid water is circulated to both of these compartments by semi-closed loops. Makeup water to compensate for electrolysis, chemical reaction, and electro-endosmosis is provided to those loops by water makeup tank component 4 (TANKG). Flow to this tank is provided by water feed tank component 3 (TANKG).

Flow in the semi-closed cathode loop is circulated by pump component 18 (PUMP). Water entering the cathode compartment is electrolyzed to form H_2 and $\overline{OH}$ ions. The $\overline{OH}$ ions migrate across a semi-permeable membrane into the absorber compartment. The effluent stream from the anode compartment flows to heat exchanger/water separator components 14 and 31 (ANYHX). Hydrogen separated from this stream is pumped by compressor component 15 (FAN) to accumulator component 16 (TANKG). The water separated is combined with makeup water at component 17 (LIQMIX) and recirculated. Cooling fluid to the condenser/water separator is provided by component 9.

The semi-closed water loop for the anode compartment is similar to that for the anode compartment. Water circulated by component 20 (PUMP) is electrolyzed to form O_2 and H^+ ions. O_2 is separated from the anode effluent in heat exchanger/

water separator components 21 and 29 (ANYHX). Makeup water enters the loop at component 19 (LIQMIX). O_2 separated is transferred by component 22 (FAN) to O_2 accumulator component 23 (TANKG).

2.7.3 Sample Problem

Description -

A sample problem was prepared for the subsystem shown in Figure 2.7-3 and described in the previous subsection. The module is sized for a six-man space station. The performance characteristics of the unit were scaled up from results presented in reference 7.1 for a three-man subsystem.

Assumptions -

1. Gas from Cabin (Air)

Flow		
Dry CO_2 free constituents	204.40	lb/hr
CO_2	1.237	
H_2O vapor	1.40	
Total		
Relative humidity	38%	
CO_2 partial pressure	3.0 mmHg	
Temperature	75°F	
Pressure	760 mmHg	

2. Humidifier

Water flow rate	0.55 lb/hr
Desired relative humidity	50%

3. Sweep Fluid Flow

Fluid	water
Flow rate	200 lb/hr
Temperature	75°F

4. O_2 Accumulator

Volume	2.0 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr-°F
Initial pressure	20.0 psia
Initial mass fraction	1 fraction

5. CO_2 Accumulator

Volume	2.0 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr°F
Initial pressure	20.0 psia
Initial mass fraction	1 fraction

6. Water Feed Tank

Volume	2 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr°F
Initial pressure	14.7 psia
Initial mass	1.0 fraction
Estimate flowout of tank	0.658 lb/hr

7. Water Makeup Tank

Volume	0.15 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr°F
Initial pressure	14.7 psia
Initial mass	1.0 fraction

8. Subsystem Blower Characteristics

Heat dissipated into process gas	50 watts

9. Anode Loop Pump

Heat dissipated into circulating fluid	10. Btu/hr
Water circulation rate	64 lb/hr

10. Cathode Loop Pump

Heat dissipated into circulating fluid	10. Btu/hr
Water circulation rate	64 lb/hr

11. O_2 Compressor

Heat dissipated into compressed gas	5.0 watts

12. H_2 Compressor

Heat dissipated into compressed gas	5.0 watts

13. CO_2 Compressor

Heat dissipated into compressed gas	5.0 watts

14. O_2/Water Separator

O_2 split ratio	.9999
H_2O split ratio	.0100

15. CO_2/ Water Separator

O_2 split ratio	.9999
H_2O split ratio	.0100

16. H_2/Water Separator

H_2 split ratio	.9999
H_2O split ratio	.0100

17. Anode Loop Heat Exchanger

Cooling fluid type	water
Inlet temperature	50°F
Flow rate	64 lb/hr
Heat exchanger effectiveness	0.90

18. Cathode Loop Heat Exchanger

Cooling fluid type	water
Inlet temperature	50°F
Flow rate	64 lb/hr
Heat exchanger effectiveness	0.90

19. Sweep Fluid Heat Exchanger

Cooling fluid type		water
Inlet temperature		50°F
Flow rate		150 lb/hr
Heat exchanger effectiveness		0.90

20. Electrodialysis Module Characteristics

No. of stacks/module		2
No. of cell pairs/stack		40
Total stack voltage	40x5.3	212 volts
Current efficiency		128%
Current density		4.6 amps/ft^2
Effective anode area/compartment		0.72 ft^2
Relative humidity of process gas effluent		50%
Power efficiency		0.30
Module thermal capacitance		18.0 Btu/°F

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
    a. number of stacks per module
    b. number of cell units per stack
    c. current density
    d. anode area

2. When attempting to match predicted results with experimental results for the same cell configuration, the following parameters should be varified:
    a. current and voltage efficiency
    b. stack voltage and current
    c. cell dimension
    d. heat transfer characteristics

3. In the sample problem, flow code 4 was used for the streams containing gas and water vapor mixtures. Thus H_2O, O_2, H_2, and CO_2 are treated as special flows 2, 3, 4, 5 respectively. When integrating the subsystem into a larger simulation containing additional EC/LS subsystems, it may be desirable to incorporate GP0LY logic to provide a suitable interface with components using flow code 3. Thus, O_2 should be transferred to R(10), H_2O to R(6), and CO_2 to R(12).

2.8 MOLTEN CARBONATE

2.8.1 Process Description:

The molten carbonate process is an electrochemical process for reduction of CO_2 absorbed from cabin air. In the basic concept lithium is reduced at the cathode of an electrochemical cell containing a molten lithium carbonate electrolyte. The lithium reacts chemically with carbon dioxide in solution to deposit solid carbon on the cathode surface and to form lithium and oxide ions in the electrolyte. At the anode, the oxide ions are oxidized to gaseous oxygen. Experimental work at Hamilton Standard Division of United Aircraft Corporation has indicated that the electrolysis of pure molten carbonate gives satisfactory results (Reference 8.2). However, its high melting point of 735°C (1,355°F), thus high operating temperatures, requires high temperature materials and associated high heat losses. These conditions also accelerate corrosion of the equipment. A lower melting point composition with similar conversion performance was found to be a eutectic mixture containing 60 percent by volume of lithium chloride and 40 percent Li_2CO_3. This eutectic mixture has a melting point of 507°C (943°F). The basic concept for the cell is illustrated in Figure 2.8-1.

The molten carbonate process, by accepting air directly from the cabin and reducing its CO_2 to carbon and oxygen, does not require the CO_2 concentration or water electrolysis units needed in other CO_2 management concepts. One of the main design problems of this process concerns the phase separation between the gases and the molten salts, especially in null gravity conditions. Another problem is the removal of carbon deposited on the cathode. Molten carbonate units may use disposable cells that are discarded after a specified quantity of carbon has been deposited on the cathode (Reference 8.2). A porous matrix, made of sintered magnesium oxide, is used as the cathode. When wetted by the melt, a stable interface is formed in the matrix because of capillary surface tensions. The matrix should be dense enough to hold the electrolyte in place under all gravity conditions, yet sufficiently porous to allow ion mobility and an efficient process. A screen (the anode) surrounds the electrolyte and the matrix. The anode screen and cathode matrix are held together by a metal diaphragm which deflects to accommodate the carbon deposited in the matrix.

<u>Cell Details</u> -

Figure 2.8-1 is a schematic of a molten carbonate electrolyte cell. Electrolytic and chemical reactions at the electrodes are shown on the figure. The net electrolytic reaction is

$$4\,Li^{+} + 2O^{=} \rightarrow 4\,Li + O_2$$

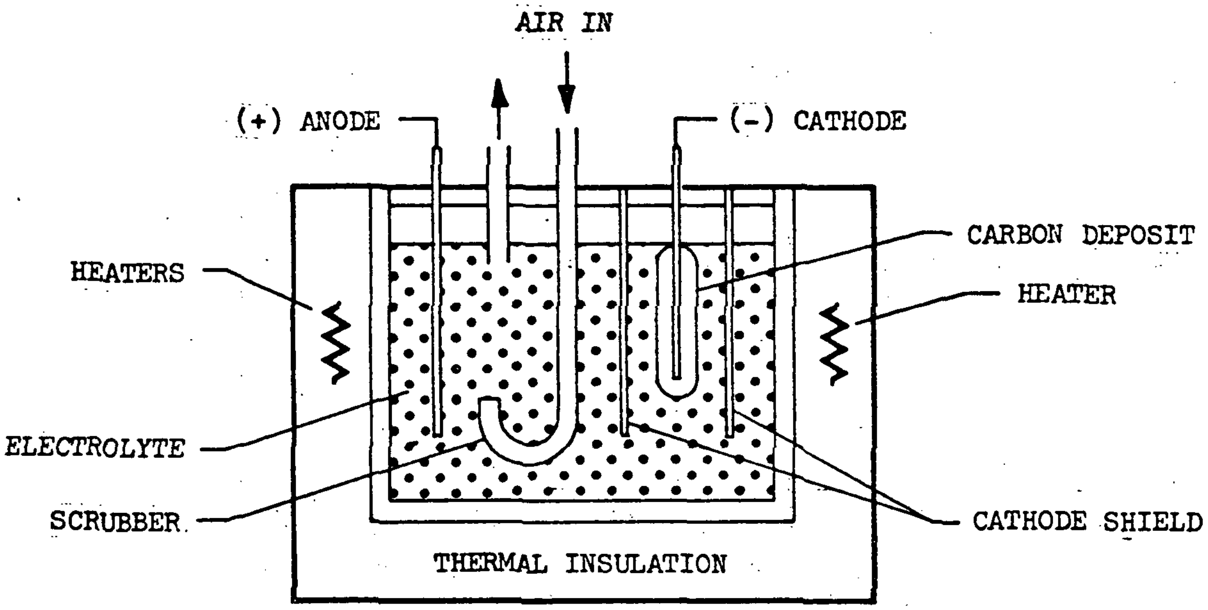


FIGURE 2.8-1 MOLTEN CARBONATE CELL

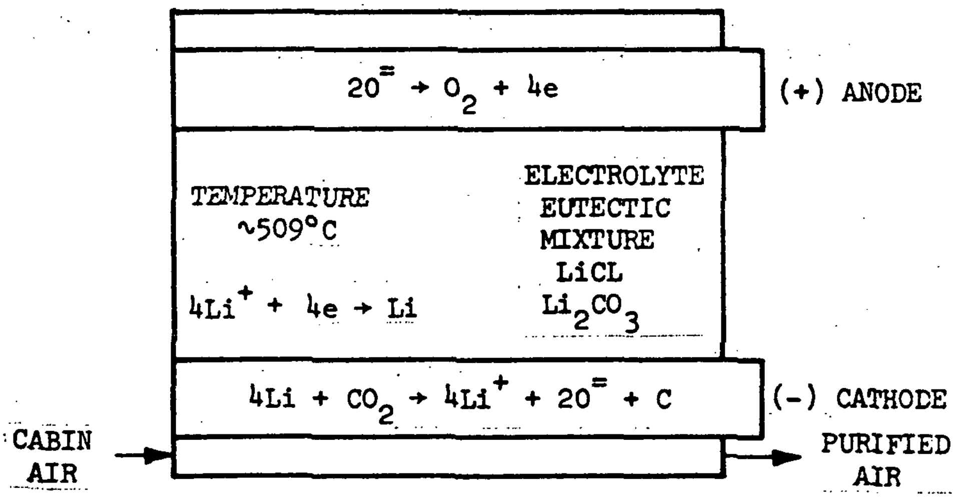


FIGURE 2.8-2 SCHEMATIC OF CELL REACTIONS FOR MOLTEN CARBONATE CELL

The theoretical cell voltage including CO_2 partial pressure gradient effects is

$$E = 1.025 - \frac{RT}{4F} \ln \frac{P_{CO_2,C}}{(PO_{2,}a)(PCO_2{}^2a)}$$

This voltage applies to a cell where water vapor reactions have been eliminated by pre-drying the cabin air prior to entering the cell. Actual required cell voltage will be higher due Joule heating losses and electrode overvoltage.

The required electrolysis current assuming 100% current efficiency is given by Faraday's law

$$I = 1100 \frac{\text{amp-hours}}{\text{lb}_{Co_2}}$$

Other reactions will occur in the cell under certain conditions. The cathode region must be shielded to prevent CO_2 from reacting with deposited carbon to form carbon monoxide (CO) since this gas is toxic if generated in significant amounts. Another possible side reaction is the hydrolysis of LiCl to form HCl. Experimental results indicate that this side reaction may be ignored.

The level of water vapor in the gas feed can have a significant effect on cell reactions. For feeds with high water vapor pressure, the oxide ion ($O^=$) concentration is inversely proportioned to the water vapor pressure. For a feed with little water vapor, the oxide ion concentration is inversely proportional to the carbon dioxide partial pressure. Since the main function of the cell is to decompose CO_2, water vapor partial pressure of the electrolyte must be made equal to the vapor in the process gas.

Water vapor pressure level also has an effect on cell voltage. At a given water vapor level, the potential between the cell electrodes will vary linearly with the logarithm of CO_2 pressure ratio between the electrode. The slope of this relationship was found to change when the level of water vapor in the feed goes from a relatively small amount to a relatively high amount.

Methane and hydrogen contamination also have been detected at the cathode. These gases may form due to side reactions involving water vapor and the carbon deposited on the cathode. These reactions provide an additional reason for cathode shielding to prevent intermixing of these contaminate gases with the purified gas leaving the cell.

Contamination of oxygen generated at the anode with CO_2 may occur if there is insufficient ionic diffusion to replenish oxide ions oxidized. Where ionic diffusion is insufficient chemical equilibrium will be shifted to generate CO_2 and the required oxide ions form $CO_3^=$. This adverse reaction may be eliminated by limiting the current density to a value which allows sufficient ionic diffusion.

Several alternate compositions have been investigated for the melt (Reference 8.2). Melts using sodium, potassium or barrium salts in place of lithium, and lithium fluoride in place of lithium chloride are examples of alternatives studied. Generally, the alternatives yield inferior performance. However, the optimum melt composition probably is not defined at this time.

2.8.2 Simulation of Concept

Figure 2.8-3 illustrates the components and subroutines required for simulating a molten carbonate concept. The concept illustrated shows a silica gel bed for predrying the process gas. While elimination of water is not a requirement, some means is required to regulate inlet gas water vapor partial pressure to match the electrolyte water vapor pressure. A humidifier also could be used to achieve this control.

The cabin air process gas is circulated through the subsystem by blower component 2 (FAN). Air then flows to valve component 8 (SPLIT) where a portion is allowed to bypass the subsystem. Flow then passes through silica gel bed component 3 (ADSORB). Cooling fluid from component 12 is used to remove heat generated by absorption of water vapor. Component 3 and 7 operate in a cyclic fashion with one adsorbing while the other is desorbing. The source of liquid flow to these components changes as the components switch operating modes. After being dried in the silica gel bed, air flows to valve component 13 (SPLIT) which regulates the amount of air flowing to regenerative heat exchanger component 4 (ANYHX). The heat exchanger serves the dual function of preheating process air above the freezing point of the carbonate cell melt and of cooling outlet air sufficiently before return to the cabin.

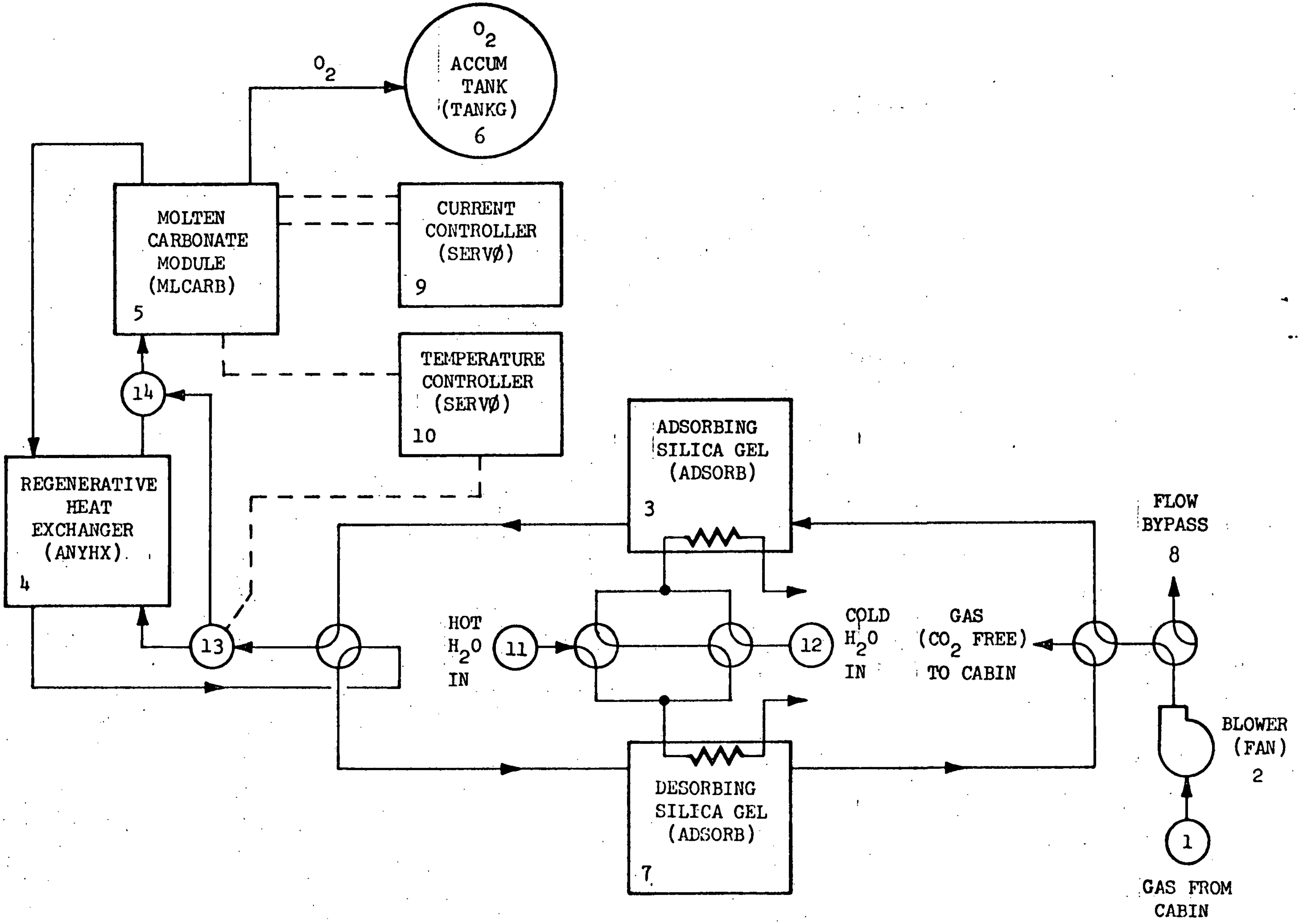


FIGURE 2.8-3 G189A SIMULATION OF MOLTEN CARBONATE CONCEPT

Automatic controller component 10 (SERVO) is used to control cell temperature by regulating the amount of process gas bypassing the regenerative heat exchanger. Cell internal heat generation will vary with fluctuations in cell current and voltage. These fluctuations arise from regulation of cell operating conditions in response to cabin CO_2 concentration. Another automatic controller , component 9 (SERVO), is used to control cell current. Since CO_2 generation is a function of metabolic activity in the cabin, precise current control is necessary to match CO_2 decomposition with the generation rate. Both controllers have "proportional position" controller action.

Process gas passes into molten carbonate component 5 (MLCARB) where absorption and reduction of CO_2 occurs. The oxygen generated is collected in accummulator component 6 (TANKG) for use by the atmospheric supply subsystem. The purified process air passes back through regenerative heat exchanger component 4 to desorbing silica gel component 7 (ADSORB). Water vapor previously absorbed is driven off by heat supplied by heating fluid from component 12 . Having been re-humidified, the purified air stream then returns back to the cabin.

2.8.3 Sample Problem

Description -

A sample problem was prepared simulating the molten carbonate concept illustrated in Figure 2.8-3 and described in the previous subsection. The cell module which is sized for 6 men is assumed to consist of 19 cells connected electrically in parallel. The temperature controller has a set point of 1022 for cell temperature with a throttling range of 950 to 1100°F. The current controller has a set point of 0.35 mm Hg with a throttling range of 25 to 35 amps. This corresponds to a CO_2 90% removal efficiency for the cell.

Assumptions -

1. Gas from cabin (air)

Flow

Dry - CO_2 free constituents	81.03 lb/hr
CO_2	.492 lb/hr
H_2O vapor	.766 lb/hr
	82.288

Relative humidity = 50% ∿ 0.0094 lb H_2O/lb dry air
CO_2 partial pressure = 3.0 mm Hg
Temperature = 75°F
Pressure = 760 mm Hg

2. Adsorbing/Desorbing Silica Gel Bed

Heat exchanger effectiveness	0.85
Average steady state bed loading	.05 lb H_2O/lb dry bed
Heat of adsorption (water vapor)	1062 + .432 T (°F)
Bed frontal area	1.0 ft^2
Bed length	1.8 ft

Superficial surface area per volume bed	507 ft^2/ft^3
Void fraction of the packed bed	0.4
Specific heat of adsorbent	.22 Btu/lb-°F
Bulk density of adsorbent	45 lb/ft^3
Mass transfer coefficient:	
during absorption	.01 $lb/hr\text{-}ft^2$ mm Hg
during desorption	
Mass of coolant in heat exchanger	1 lb
Initial conditions (absorption)	
H_2O loading	.05 lb/lb
Bed temperature	75 °F
Adsorbate exit partial pressure	1.0×10^{-12} mm Hg
Initial conditions (desorption)	
H_2O loading	0.1 lb/lb
Bed temperature	75. °F
Adsorbate exit partial pressure	20. mm Hg
Cooling fluid data (absorption)	
Inlet temperature	38°F
Specific heat	1.0 Btu/°F
Viscosity	3.90 lb/ft-hr
Flowrate	100. lb/hr
Fluid: water	
Heating fluid data (desorption)	
Inlet temperature	200°F
Specific heat	1.0 Btu/°F
Viscosity	.740 lb/ft-hr
Flowrate	100. lb/hr
Fluid: water	

3. Blower Characteristics

Heat dissipated into air	60 watts

4. Regenerative Heat Exchanger Characteristics

Effectiveness	.97
Design outlet temperature, primary side	550°C (1022°F)

5. Molten Carbonate Cell

UA between surface of insulation and ambient gas	0.5 Btu/hr-°F
Ambient wall temperature	70°F
Thermal conductance of insulation	.5 Btu/hr-°F
Cell current	30.0 amps
Cell voltage	2.35 volts
Cell thermal capacitance	75. Btu/°F
Cell temperature (estimated)	1022. °F
Number of parallel cells	19

6. Oxygen accumulator Tank

Volume	2.0 ft^3
Overall thermal conductance to surroundings	2.0 Btu/hr-°F
Initial pressure	14.7 psia
O_2 use rate	0.5 lb/hr
Initial mass oxygen	1. fraction

7. Current controller

Action: proportional position

Dead band: .01 mm Hg

Set Point: 0.35 mm Hg

Throttling range: 25-35 amps

Sensor time constant: 0.1 sec

Maximum speed of FCE: 0.1 sec^{-1}

8. Temperature Controller

Action: proportional position
Dead band: 1°F
Set point: 1022°F (550°C)
Throttling range: 950 to 1100°F
Sensor time constant: 0.1 sec
Maximum speed of FCE: 0.1 sec^{-1}

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
    a. number of cells per module
    b. cell current
    c. electrode area
2. When attempting to match predicted results with experimental results for the same cell configuration, the following parameters should be varified:
    a. current and power efficiency
    b. cell dimensions
    c. heat transfer characteristics
    d. cell current and voltage

2.9 MEMBRANE DIFFUSION

2.9.1 Process Description:

Concentration by membrane permeation is a mass transfer process accomplished by a partial pressure difference and selective diffusion. The degree of separation is dependent on the difference in transfer rates of the component gases across the membrane. Membranes have been developed that yield a separation of 99% pure CO_2.

The membranes are packaged in multiple layers with intervening backing screens. The supply gas or "feed" gas is forced laterally through every other screen and "sweep" gas for removing outlet CO_2 flow is forced through the alternate screens. The individual parallel passages for feed and sweep gas streams in the multiple layer configuration are manifolded together. Figure 2.9-1 from Reference 9.8 shows a representative multiple layer configuration. Figure 2.9-2 is a schematic representation of the design of a module.

Low pressure steam (15 mm Hg) is used as the sweep gas. The outlet CO_2 is absorbed in the steam. The CO_2 is removed from the water vapor in a condensing heat exchanger and it is subsequently pumped into an accumulator or is evacuated to space. The condensed water is revaporized for use as sweep gas.

The critical parameter is the permeability which has units of:

$$[\text{Perm}] = \left[\frac{(\text{volumetric flow (STP)}\ )\quad(\text{thickness})}{(\text{time})\ (\text{area})\quad(CO_2\ \text{pressure differential}}\right]$$

Increasing the CO_2 pressure differential reduces the mass transfer area and this, in turn, directly reduces the weight and volume of the packaged module. In Reference 9.8 the CO_2 inlet pressure was increased from 7.6 mm Hg to 35.8 mm Hg through compressing the feed flow total pressure from 258 to 760 mm Hg. This procedure is feasible when the cabin pressure is much less than 1 atmosphere. The membranes tested in Reference 9.8 were subjected to pressure differentials of 1 atmosphere or less. Some difficulties in maintaining satisfactory seals, preventing pinholes leaks, and preventing scoring of membranes by the backing screens were experienced at pressure differentials of 1 atmosphere. The bubble point for the membranes was over

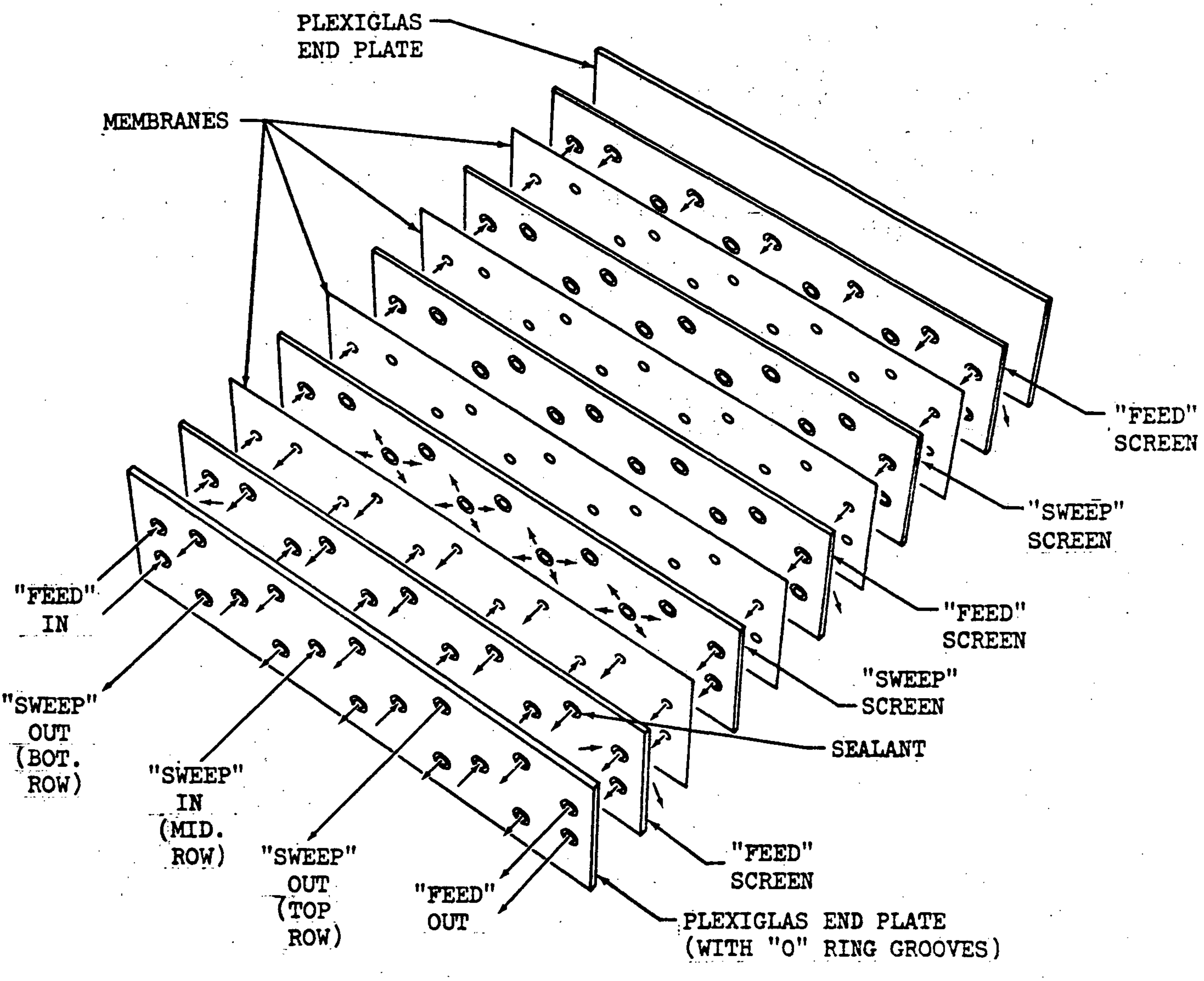


FIGURE 2.9-1 MEMBRANE MODULE

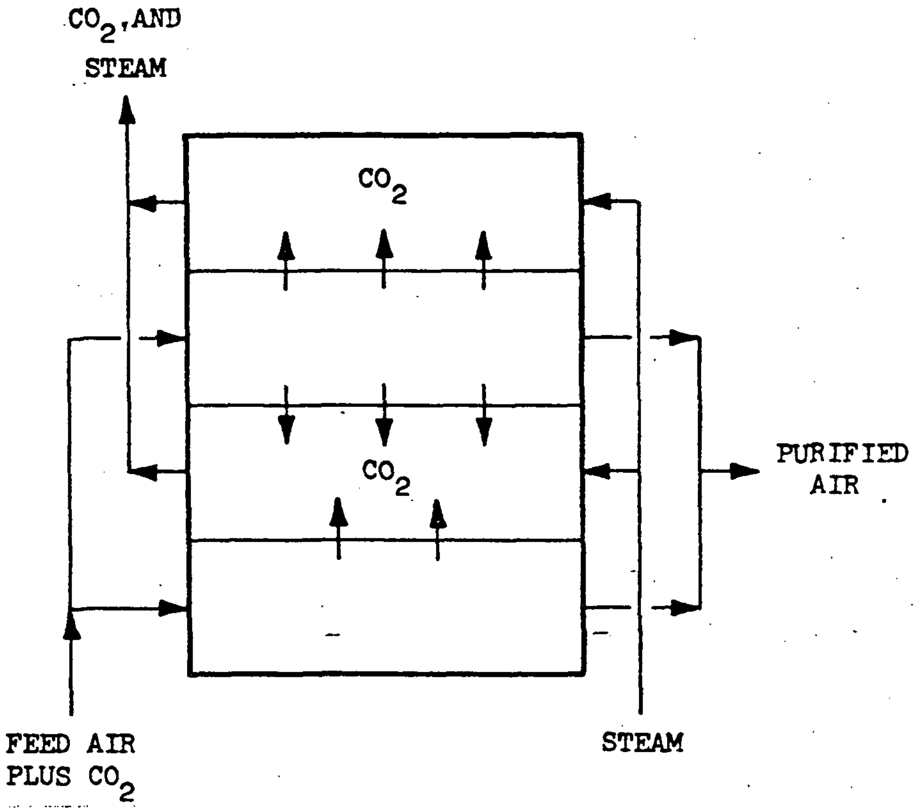


FIGURE 2.9-2 MEMBRANE DIFFUSION MODULE

30 psi so 15 psi pressure differential was considered to be safely below the maximum allowable pressure differential. When cabin pressures are high the CO_2 pressure could again be increased by compressing the feed gas providing a membrane can be developed which would successfully withstand the resulting pressure differential. This technique would require that the membrane module be constructed as a pressure vessel. Preliminary calculations have indicated that for total pressures up to 10 atmospheres the weight of the pressure shell is only of the order of 10% of the basic membrane module.

2.9.2 Membrane Description and Cell Details

The degree of separation (CO_2 removal) is dependent on the difference of transfer rates and pressure differential of the constituent gases across the membrane. The rate controlling mechanism is a flow conduction process involving the adsorption and solution of a constituent, diffusion of solute through the barrier under a concentration potential (pressure differential), and desorption and evaporation of solute from the surface. One well known membrane is silicone rubber which combines high CO_2 permeability and high CO_2/O_2 separation factor (ratio of CO_2 permeability to O_2 permeability) of 5.5. However, for a practical CO_2 removal system, this separation factor is inadequate.

Highly effective, immobilized liquid membranes that yield a CO_2/O_2 separation of 99 + % were developed. Initially, an immobilized liquid film was made by containing a 1 to 2 mil porous Dacron mat impregnated with saturated $CsHCO_3$ solution backed by silicone rubber membranes. However, it was found that the caustic $CsHCO_3$ solution attacked the silicone rubber causing pinholes to develop, resulting in cross-membrane leaks and a low separation factor. In place of the rubber membrane, a microporous, hydrophobic film manufactured under a trade name "Solvinert" by Millipore Corporation was found to be effective in providing a method for immobilizing the liquid film. The Solvinert film is unaffected by the aqueous salt solutions used and the bubble point of liquid impregnated silicon (the pressure required to blow the liquid through the pores of the film) was in excess of 30 psi.

Since the membrane consists of saturated $CsHCO_3$ solution backed by the Solvinert filters, it is desirable to operate the sweep side of the package with a water vapor sweep stream at a total pressure equal to the equilibrium vapor pressure of the aqueous solution. This enables recovery and reuse of both constituents of CO_2-H_2O sweep stream, a necessity for long term missions. In addition, the air at the feed side should be water saturated to prevent the drying of the feed side of the membrane and pinhole leaks developing.

A CO_2 scrubber using the Solvinert membranes with a projected packaging density of 440 Ft^2/Ft^3 was developed for the Air Force Flight Dynamics Laboratory. The membranes were packaged in multiple layers with intervening backing screens. The supply gas or "feed" gas is forced laterally every other screen (Figure 2.9-1). A summary of membrane and screen details is given below:

Membranes:	Millipore Corporation "Solvinert" films Microporus, hydrophobic film, pore size 20μ porosity 70%, thickness .005 in, impregnated with aqueous $CsHCO_3/NaAsO_2$ solution: 6.4 M $CsHCO_3$, 99.9% pure .25 M $NaAsO_2$ 1% to 2% by volume polyethylene glycol
Feed Gas Screens:	PE 400 polyester monofilament screens, thickness .013 in., 400 mesh openings, 47% open area
Sweep Gas Screens:	PE 1120 polyester monofilament screens, thickness .024 in., 120 mesh openings, 58% open area

2.9.3 Simulation of Concept:

The G-189 simulation of the CO_2 removal system using the membrane diffusion concept is shown schematically in Figure 2.9-3. Inlet air, defined by a dummy component (component 1) is forced to a condensing heat exchanger for humidity control (component 3) by a high pressure fan simulated by subroutine FAN, Component 2, simulating a compressor. As the air passes through the membrane module (component 4), a portion of the CO_2 permeates the membrane to the "sweep" side of the module which is using steam as the sweep gas. The purified air is returned to the cabin. The CO_2 that permeates through the membranes is pumped along with the sweeping water vapor stream to a condenser-separator, component 6, for H_2O/CO_2 separation.

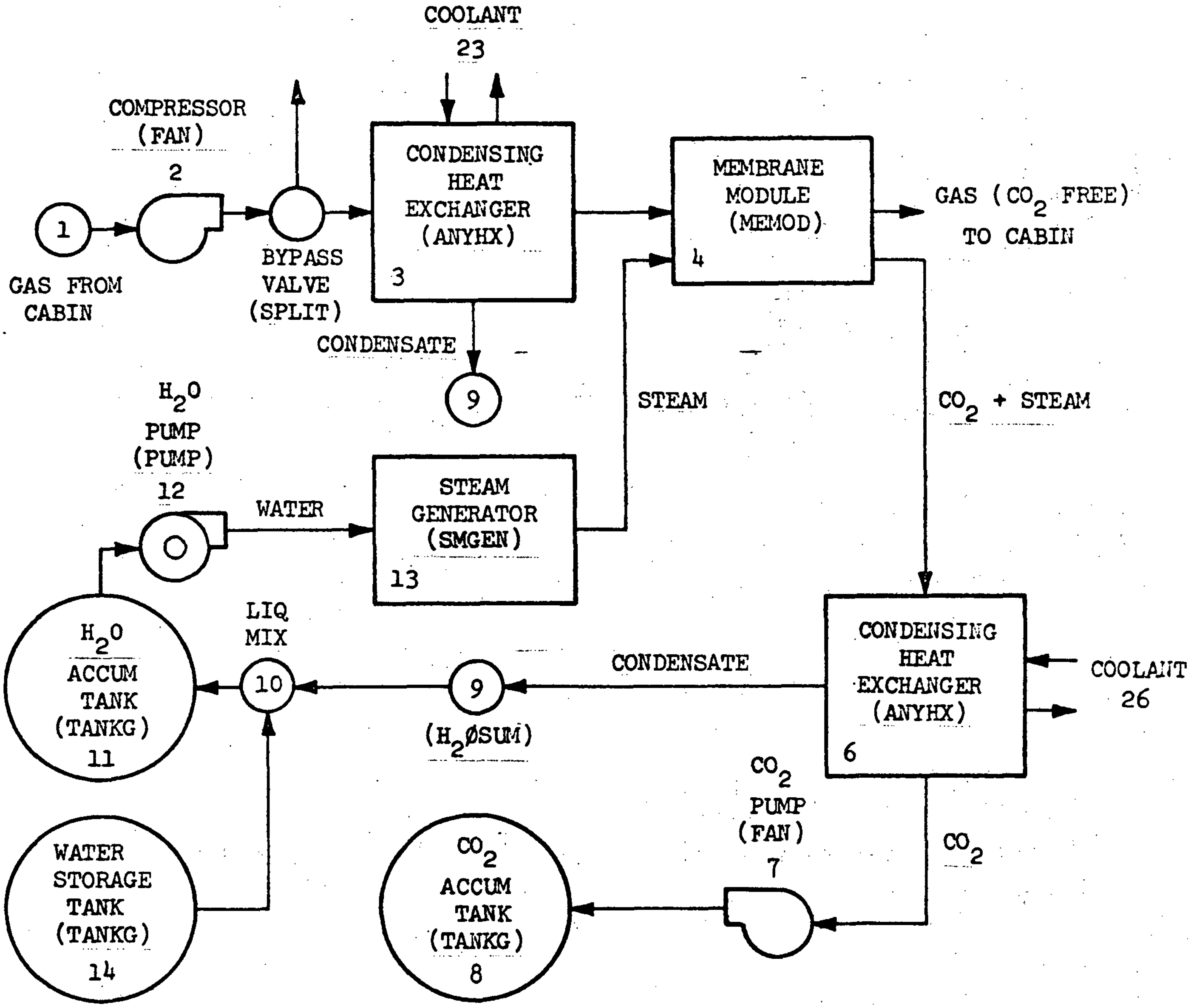


FIGURE 2.9-3 G189A SIMULATION OF MEMBRANE DIFFUSION CONCEPT

The CO_2 is then pumped by component 7, simulated by PUMP, to the CO_2 accumulator which is simulated by subroutine TANKG, component 8.

The condensed water from both condensing heat exchangers, components 3 and 6, is removed and summed by the new subroutine, H20SUM, "The Water Summation Subroutine". This subroutine sums condensate flow from up to 5 condensing heat exchangers and determines the mix temperature of total flow.

A method for adding makeup water for this CO_2 removal system is provided by component 10, LIQMIX, by providing for H_2O flow from the water supply subsystem. The makeup water from water supply will be added as required, to the H_2O accumulator, component 11, to maintain a relatively constant H_2O level in the H_2O accumulator. The required rate of addition will be determined by GPOLY logic. Component 12, simulating an H_2O pump, provides constant water flow from the accumulator to the steam generator, component 13. The steam generator is simulated by a new subroutine SMGEN. SMGEN is used to supply superheated steam for use in various EC/LS subsystems such as the CO_2 removal system utilizing the membrane module.

A new subroutine was written to simulate component 4, membrane module. This new subroutine, MEMOD, models the mass and thermal balance of a membrane module which would have gases of different concentrations flowing through the modules two sides.

2. 9.4 Sample Problem

Description -

A sample problem simulating major components of the CO_2 removal system utilizing the membrane diffusion concept has been prepared for the performance analysis of the system. The inlet conditions of the sample problem, shown schematically in Figure 2.9-3, are defined by a dummy component simulating cabin air flow to the system. A compressor is used to pressurize the air to 30psi in order to provide sufficient CO_2 pressure differential to obtain adequate separation. The data defined by the dummy component include total flow, cabin temperature,cabin pressure, non-condensable, condensable vapor flow, entrained liquid flow, non-condensable specific heat, non-condensable molecular weight, oxygen flow, diluent (N_2) flow, and CO_2 flow. The input values to the first component are derived from assumptions defining cabin air conditions. The inlet conditions along with performance of the whole system are used in deriving the design parameters of individual components of the system.

Assumptions -

1. The cabin air conditions are as follows:

Dry bulb temperature	70°F
Wet bulb temperature	60°F
Cabin pressure	14.7 psi
Partial pressure CO_2	3.0 mmHg
O_2 pressure	3.1 psi
CO_2 generation/removal rate per men	.1 lb/hr-man
Number of men	6

Reference 9.8 provides data for a "Solvinert" film membrane module, giving CO_2 removal rate of a one man system for the following operating conditions.

Feed flow (Air)	30 liters/min
Temperature	80. °F
Pressure	760 mmHg
CO_2 pressure	22.8 mmHg

Sweep flow (steam)	60 liters/min
Temperature	80°F
Pressure	26 mmg/Hg
Membrane Area	21 sq-yds.

Computing the removal efficiency of the system from the above data we determine the required volumetric flow (2490 ft^3/hr) from which we compute the flows of individual constituents to the system defined as inputs to component #1.

Total flow (lb/hr)	184.64
Temperature (°F)	70.
Upstream duct outlet pressure (PSI)	14.7
Component outlet pressure (PSI)	14.7
Non-condensable flow (lb/hr)	182.60
Condensable vapor flow (lb/hr)	2.041
Non-condensable specific heat (Btu/lb-°F)	.24
Non-condensable molecular weight (lbs/mole)	28.97
Oxygen flow (lbs/hour)	48.96
Diluent (N_2) flow (lbs/hour)	138.0
CO_2 flow (lbs/hr)	1.103

2. The air compressor, simulated by subroutine FAN, pressurizes the air to 30 psi via GPOLY logic. The pressurization process is assumed to be approximately isentropic and with consideration for heat loss to surroundings the outlet temperature is raised accordingly. No other inputs are required for the component.

3. Process Air Condensing Heat Exchanger Characteristics:

Overall UA (BTU/hr-°F)	75.
NTU (Max)	5.0
Design outlet temp, primary side (°F)	80.0
Tolerance for design temp, primary side (°F)	5.

The secondary flow is provided by component #23 with inlet conditions defined by the following.

Flow rate (lb/hr)	60.
Temperature (°F)	38.
Upstream duct pressure (psi)	15.0
Component outlet pressure (psi)	15.0

The physical properties of the coolant (water), are listed as follows:

Specific heat (Btu/lb-°F)	1.0
Viscosity (lb/hr-ft)	3.6
Density (lb/Ft^3)	62.4
Molecular weight (lb/mole)	18.0
Conductivity (Btu/hr-ft-°F)	.325

The physical properties listed above also apply to coolant flow from component 26 which is used to provide secondary flow to component 6.

4. CO_2 Concentrator (Membrane Separator) Characteristics

The separation, and thereby removal of CO_2 from cabin air stream is accomplished by component #4, the membrane module. The component is simulated by the new subroutine MEMOD with the required input being as follows:

Number of membranes	940
Heat loss to surrounding data:	
Ambient gas temperature (°F)	70.
Thermal conductance between surface and ambient (Btu/hr-°F)	1.3
Ambient wall temp (°F)	60.
FA factor for radiation conductance (Ft^2)	6.
Structure temp (°F)	60.
Conductance between module and structure	12.
Steady state data input required	
Membrane area per cell (Ft^2)	2.
Thickness	.005
CO_2 permeability $\frac{(Ft^3/hr)\ (inches)}{(Ft^2)\ (mmHg)}$	1.2×10^{-5}
Transient data input	
Frontal area, primary side (Ft^2)	.1
Frontal area, secondary side (Ft^2)	.1
Module length (Ft)	2.
Thermal capacitance of module shell, Btu/°F	12.0

5. CO_2/H_2O Condenser/Water Separator Characteristics

Overall UA (Btu/hr-°F)	460.
NTU (Max)	5.
Primary outlet design temp (°F)	42.
Design outlet temp tolerance (°F)	2.

The secondary flow to the condensing heat exchanger is provided by a dummy component, 26, simulating coolant flow to the heat exchanger. The flow from component 26 is specified as follows:

Flow rate (lb/hour)	270.
Temperature (°F)	35.
Pressure (Psi)	15.

6. CO_2 Accumulator Characteristics

Total fluid weight in tank (lbs)	.5
Fluid temp in tank (F°)	70.
Fluid volume in tank (Ft^3)	1.
Fluid pressure in tank (Psi)	14.7

7. Steam Generator Characteristics.

Flowrate (lb/hr)	6.5
Pressure	1.0
Temperature (°F)	120
Desired degrees of superheat (°F)	20.

Special Notes –

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
    a. number of membrane cells
    b. membrane area per cell

2. When attempting to match predicted results with experimental results for the same cell configuration, the following parameters should be varified:
    a. constituent permeabilities
    b. cell dimensions
    c. heat transfer characteristics

2.10 MECHANICAL FREEZOUT

2.10.1 Process Description

This process precipitates out the CO_2 from cabin air that is passed through a heat exchanger. In its simplest form, cabin air is passed through a heat exchanger which removes thermal energy thus reducing the temperature. At some point, the CO_2 will begin to precipitate and the noncondensable cabin air which will become relatively free of CO_2 may then be recycled. In the range of CO_2 partial pressures encountered, carbon dioxide begins to precipitate at -125°C ($PPCO_2$ = 5.0 mm Hg, saturated) and its removal will practically be total at -140°C ($PPCO_2$ = 0.43 mm Hg, sat.). Water is assumed to be completely removed using the silica gel bed upstream of the precipitation channel and will not interfere with either the precipitation or sublimation of the carbon dioxide.

Several carbon dioxide removal systems utilizing the freezout concept have been proposed; however, only the two more practicable systems will be presented here. The first system, shown in Figure 2.10-1, uses precipitator/sublimator coupled to a very cold space radiator to remove the CO_2; the second system, shown in Figure 2.10-2, requires the use of a refrigeration system. The space radiator and the refrigeration system are necessary in both cases for thermal energy removal to account for the inefficiencies of the regenerative heat exchangers that are being utilized and the heat flux from the surroundings into the system. Both systems use a water condenser for humidity control, and a silica gel bed for predrying the cabin air before passing it through the regenerative heat exchanger. It is imperative that the air be dried prior to its passage into the regenerative heat exchanger to prevent the buildup of frost which would deteriorate its performance.

The CO_2 removal system which utilizes the precipitator sublimator, hereby referred to as the P/S system, will be considered to be an open system. Its operation predicates the simultaneous precipitation and sublimation of CO_2 frost. For sublimation to occur, the CO_2 frost must be exposed to the vacuum of space. In the simultaneous precipitation and sublimation, the heat of

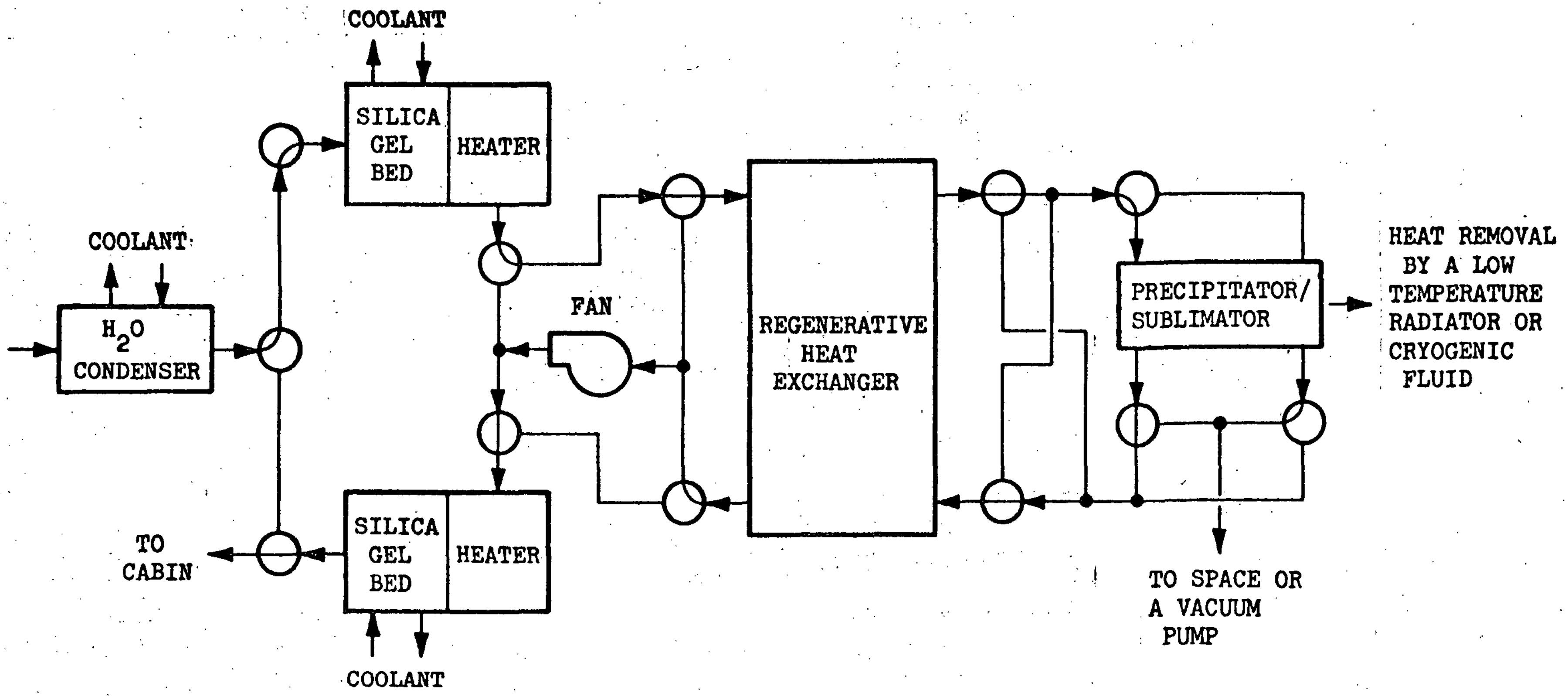


FIGURE 2.10-1 MECHANICAL FREEZE-OUT SYSTEM, NON-RECOVERABLE CO_2

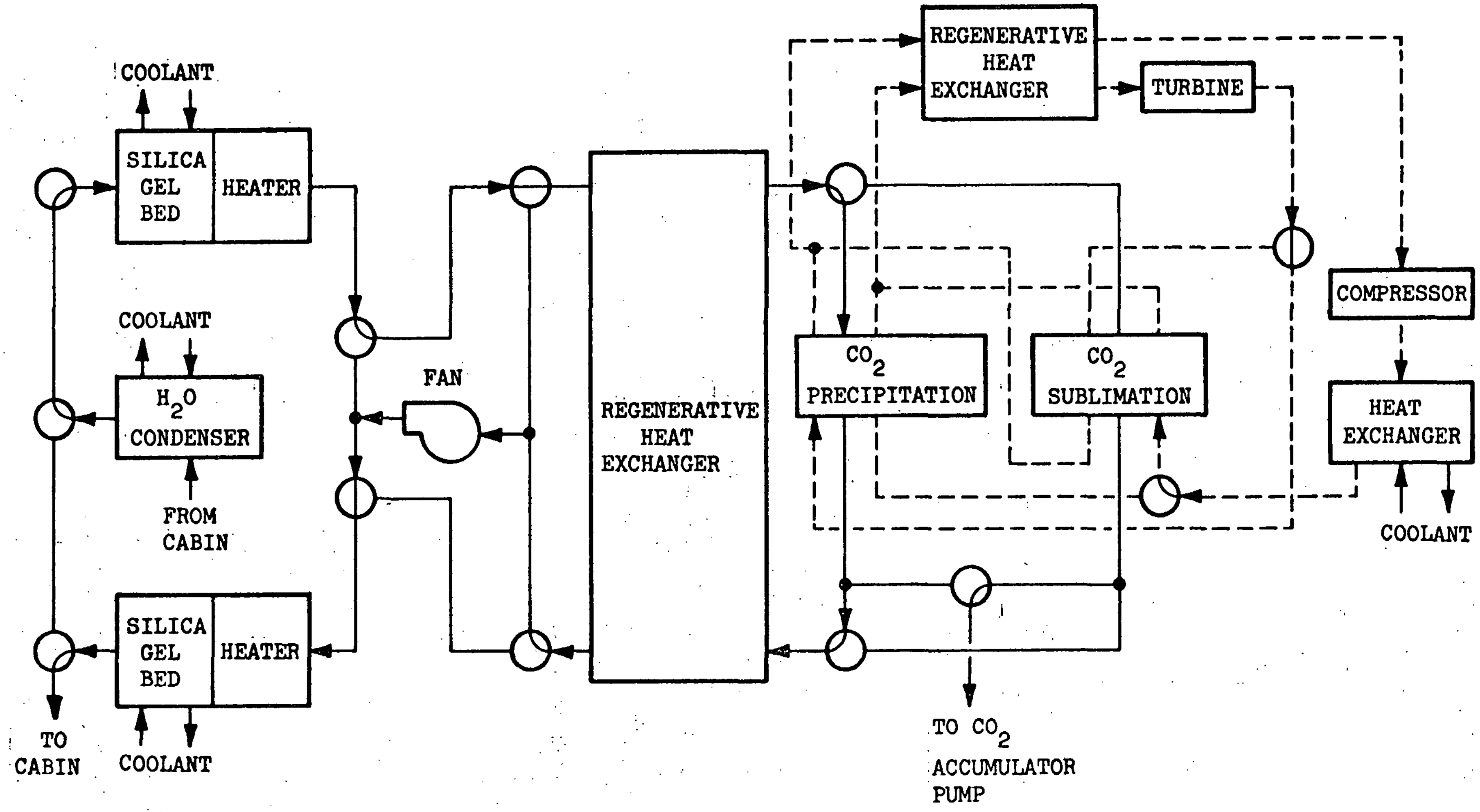


FIGURE 2.10-2 MECHANICAL FREEZE-OUT SYSTEM, RECOVERABLE CO_2

precipitation supplies the thermal energy required for the sublimation to space. However, to account for the inefficiency of the regenerative heat exchangers and the heat influx into the CO_2 removal system due to pipe connectors and supports, a method for removal of thermal energy must be included. Two methods for the removal of thermal energy have been proposed. The first method described in Reference 10.6 through 10.7 uses cryogenic O_2, N_2 or H_2 to remove the heat to make the system operational. The second method employs a low temperature radiator to reject the heat from system to drive the precipitation sublimation process. This method, described in References 10.1, 10.5, and 10.6, relies on the ability to design a radiator that operates at -250°F which presently does not appear feasible.

The Mechanical Freezout System-Recoverable CO_2, shown in Figure 2.10-2, uses a refrigerant to chill the cabin air flowing through the precipitation channel. This type of system minimizes the total vehicle weight penalty at the expense of an increase in required power input. For long-duration space missions, studies have shown (Reference 10-7) that the reversed Brayton-cycle system offers the most desirable method for heat removal. The reversed Brayton cycle system offers the following advantages with respect to the other systems:

Employs a single phase fluid and thereby its operation is simpler and more flexible than the Claude cycle.

The entire expansion occurs in a turbine, thus allowing high temperature operation which is more efficient.

In addition, the system has potential for long-duration maintenance-free operation.

The use of the hotter compressed gas in the refrigerant system to sublime the CO_2, as shown in Figure 2.10-2, affords a method for the recovery of the precipitated CO_2 without the use of deep space vacuum (thermal sublimation). In addition, more positive control of the precipitation and sublimation processes is provided.

2.10.2 Simulation of Concept

The simulation of the mechanical freezout concept is performed by dividing the subsystem into major functional components which may be mathematically modeled by G-189A component subroutines.

Figure 2.10-3 shows the G-189 component connection and definition diagram which was prepared for the analysis of the subsystem. Dummy component 1 (subroutine ALTCOM) is used to define the inlet conditions (flowrate, temperature, humidity, CO_2 partial pressure, constituency, etc.) to the subsystem.

A H_2O condenser, component 2 (ANYHX), is used in comjunction with a silica gel bed, component 3 (ADSØRB), to dry the air sufficiently to prevent H_2O freezeout in the CO_2 precipitating heat exchanger, component 6. Dummy component 12 (ALTCOM) provides the coolant to the condensing heat exchanger at a specified temperature and flowrate. The condensate is pumped by component 17 (PUMP) to a water storage tank, simulated by component 18 (TANKG).

The dehumidified air from the silica gel bed passes through a switched off heater, component 4 (ALTCOM), to regenerative heat exchanger, component 5 (ANYHX). Here the air is pre-cooled prior to entering the CO_2 precipitator. The secondary flow for this component is the effluent from the precipitator heat exchanger.

The precipitator heat exchanger, component 6, is simulated by a modified version of subroutine ANYHX. A new subroutine, CO2CP, has been added to the program to simulate the CO_2 precipitation process in the heat exchanger component. In addition to determining the amount of precipitation, this subroutine determines the effective specific heat of the process air entering and leaving the precipitator. Refrigerant flow to the precipitator is supplied by dummy component 16 (ALTCOM).

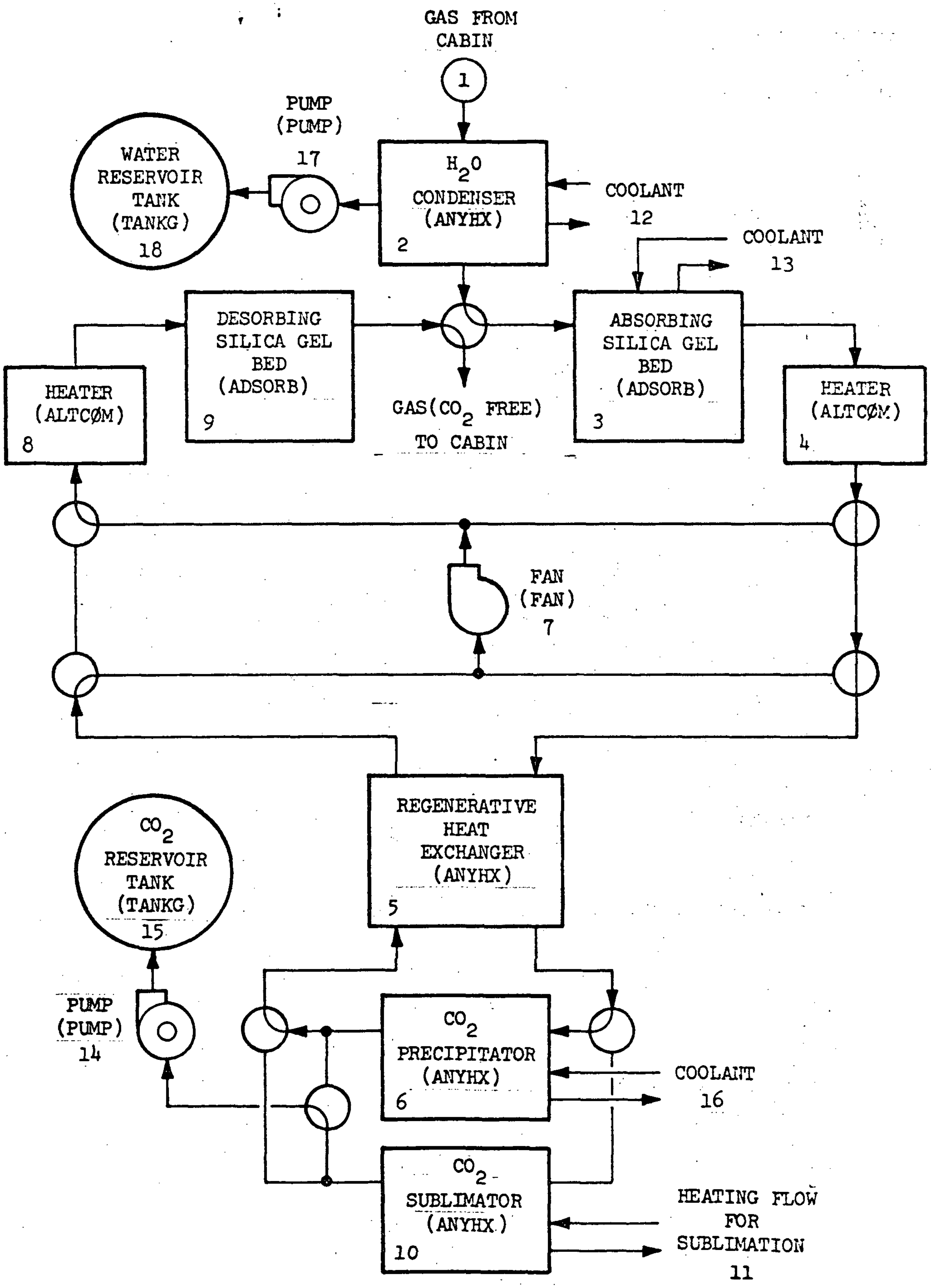


FIGURE 2.10-3 G189A SIMULATION OF MECHANICAL FREEZE-OUT

Air flow from the precipitator is circulated by fan component 7 (FAN) back through the regenerative heat exchanger to heater component 8 (ALTC0M) and desorbing silica gel bed component 9 (ADS0RB). The heater component provides the thermal energy required to force water vapor desorption in the silica gel bed.

The sublimation of CO_2 is simulated with component 10 (ANYHX). The rate of sublimation is assumed to equal the rate of precipitation in component 6. This rate, which is the difference between the flow of CO_2 in and out of the precipitator, is calculated by GP0LY logic. Dummy component 19 is used to supply CO_2 to the sublimator at a rate equal to the sublimation rate. Component 10 calculates the amount of heat absorbed in sublimating the solid CO_2. This energy is removed from heating fluid circulating through the sublimator. The heating fluid, which is assumed to be gaseous nitrogen is supplied by component 11. The CO_2 sublimated is pumped by component 14 (PUMP) to CO_2 accumulator component 15 (TANKG).

Because of the cyclic operation of the system, components 3 and 9, 4 and 8, and 6 and 10 alternately switch functions according to a pre-determined time sequence. Logic is incorporated in GP0LY to change the order of solution path, modify sources of flows, and perform other miscellaneous operations when the switch of functions occurs.

2.10.3 Sample Problem

Description -

A sample problem, simulating the major components of the mechanical freezout system, was prepared for the performance analysis of the system and to provide insight to the sizing and power requirements of the system. The inlet conditions of the sample problem are defined by a dummy component simulating cabin air flow to the system shown in Figure 2.10-3. The required inlet conditions include the following: total flow, fluid temperature, upstream duct outlet pressure, component outlet pressure, non-condensable flow, condensable vapor flow, condensable entrained liquid flow, non-condensable specific heat, non-condensable molecular weight, oxygen flow, diluent flow, and CO_2 flow. The assumptions made for determining the inlet conditions and performance characteristics of the individual components of the subsystem are presented below:

Assumptions -

1. The cabin air conditions, which define the data for component #1 are as follows:

Dry bulb temperature	70°F
Wet bulb temperature	60°F
Pressure	14.7psi
O_2 pressure	3.1psi
Partial pressure CO_2	3.5 mmHg
CO_2 generation/removal rate per man	.1 lb/hr man
Number of men	6

The weight flowrates for O_2, N_2, CO_2, and H_2O through the mechanical freezout system are derived from the required volumetric flow. The volumetric flow is calculated from the following relationship:

$$Q = \frac{W_c N \times R_{co_2} \times T}{E_p \times PPCO_2}$$

Q = Required volumetric flowrate, CFH
R_{CO_2} = Universal gas constant for CO_2, 35.12 ft/°R
T = Cabin temperature, 530°F
$PPCO_2$ = Partial pressure of CO_2, 3.0mm Hq
W_c = CO_2 generation/removal rate per man lb/hr man = 2.3 $\frac{lb}{m\text{-}day}$
N = Number of men
E_P = Precipitation efficiency, 0.9 $\equiv \frac{C_i - C_o}{C_i}$

The given inlet conditions and the computed volumetric flow were used to calculate the following items:

Total flow	111.6 lb/hr
Temperature	70.0 °F
Upstream duct outlet pressure	14.7psi
Component outlet pressure	14.7psi
Non-condensable flow	110.43 lb/hr
Condensable vapor flow	1.17 lb/hr
Condensable entrained liquid flow	0. lb/hr
Non-condensable specific heat	.24 Btu/lb-°F
Non-condensable molecular weight	28.97 lbs/mole
O_2 flow	29.35 lbs/hour
N_2 flow	80.41 lbs/hour
CO_2 flow	.66 lbs/hour

2. The required data input for component 2, a condensing gas-liquid heat exchanger are given below:

Overall UA = 93.5 BTU/hr-°F
NTU (MAX) = 3.0
Design outlet temp for primary side = 45°F
Tolerance for primary side outlet temp = ±3°F

The inlet conditions of secondary flow or coolant are as follows:

Flowrate = 270 lb/hr
Temperature = 38 °F
Upstream duct pressure = 15.0 psi
Component outlet pressure = 15.0 psi

The physical properties of the coolant (water), are listed as follows:

Specific heat	1.0 b/lb-°F
Viscosity	3.6 lb/hr-ft
Density	62.4 lb/ft
Molecular weight	18.0 lb/mole
Conductivity	.325 Btu/hr-ft-°F

These values apply to flows from components 12, 13, and 21

3. Subroutine ADSORB is used to simulate the silica gel beds, component 3,

for the adsorption of H_2O vapor from the process air. The required inputs for subroutine adsorb are as follows:

Heat exchanger effectiveness, ε	.85
Average steady state bed loading	.055 $\left\{\frac{\text{lb } H_2O}{\text{lb bed}}\right.$
Heat of adsorption (water vapor)	1062 + .432T
Adsorption bed frontal area	1.0 ft^2
Adsorption bed length	1.8 ft
Superficial surface area per volume bed	507 ft^2/ft^3
Void fraction of the packed bed	.4
Specific heat of bed material	.22 Btu/lb-°F
Bulk density of bed material	45. lb/ft^3
Mass transfer coefficient	.01 $lb/hr\text{-}ft^2mmHg$
Mass of coolant in heat exchanger	4 lbs
Init. value adsorbate gas pressure	1.0 X 10-12 mmHg
Init. value bed loading (lb adsorbate/lb bed)	1.0 X 10 -12 mmHg
Carrier gas outlet temperature	45°F
Adsorbent bed temperature	40°F
Liquid coolant outlet temperature	40°F

The coolant flow (secondary) for the silica gel beds is provided by component #13. The coolant inlet conditions are as follows:

Flowrate = 270. lb/hr
Temperature = 38. °F
Upstream duct outlet pressure = 15.0 psi
Component outlet pressure = 15.0 psi

4. No inputs are required for component 4, a turned-off heater simulated by a dummy subroutine ALTCOM. Subroutine ALTCOM passes data from component 3 to 5 unchanged.

5. Component 5, regenerative heat exchanger, is simulated by subroutine ANYHX. It is a gas-gas counterflow heat exchanger that uses the primary temperature as the criterion for sizing. The required V-array data for the regenerative heat exchanger are as follows:

Overall UA (Estimate)	210. Btu/hr-°F
NTU (Max)	5.0
Design outlet temperature, primary side	-190. °F
Tolerance for design outlet temp.	± 3.°F

The secondary flow (coolant) for the regenerative heat exchanger is supplied by the precipitator heat exchanger, component 6. Therefore, initial values of the outlet flow must be made for component 6. The values given as follows:

Total flow	109.1 lbs/hr
Temperature	-220.0 °F
Upstream duct outlet pressure	14.7 psi
Component outlet pressure	14.7 psi
Non-condensable flow	109-1
Non-condensable specific heat	.24 Btu/lb-°F
Non-condensable molecular weight	28.97 lbs/mole
Oxygen flow	29.35 lb/hr
Diluent flow	80.41 lbs/hr

6. The precipitator heat exchanger, component 6, is simulated by the subroutine ANYHX. Dry process air enters the heat exchanger at $\approx$-190°F and is chilled down to -223°F causing the precipitation of CO_2 to occur thus removing it from the gas stream. The required data are as follows:

Overall UA	35 Btu/hr-°F
NTU (Max)	3.0
Design outlet temperature, primary side	-223°F
Tolerance for design temperature	± 3°F

The coolant (Secondary) flow to the precipitator heat exchanger is provided by component 16. The flow inlet conditions are defined as follows:

Total flow	45.0 lbs/hr
Temperature	-280.0 °F
Upstream duct outlet pressure	20 psi
Component outlet pressure	20 psi
Non-condensable flow	45.0 lbs/hr
Non-condensable specific heat	.239 B/lb-°F
Non-condensable molecular weight	28.0 lbs/mole

The physical properties of the refrigerant,(cold nitrogen is assumed)are as follows:

Specific heat	.239 Btu/lb-°F
Viscosity	.036 lb/hr-ft
Density	.16 lb/ Cu ft
Molecular weight	28.0 lb/mole
Conductivity	.007 Btu/hr-ft-°F

7. The blower, component 7, which forces the air through the mechanical freezout system is simulated by subroutine FAN. The component is simulated only to the extent that heat is added to the gas stream. The required V-array input is as follows:

Heat added to gas stream	100 watts

8. The heater component 8, which is used for heating the air for desorption of the silica gel bed is simulated by a dummy component subroutine ALTCOM. The subroutine computes the outlet temperature of the gas stream due to the heat added. The required V-array input is as follows:

Heat load to cooling fluid	1535 Btu/hr

9. The desorption of silica gel beds, component 9, is simulated by subroutine ADSORB. This component has the same input data requirements as component #3 exclusing parameters that pertain to coolant flow.

10. Components 17 and 18 simulate the water pump (PUMP) and water accumulator (TANKG) respectively. The pump receives its flow from a dummy component, component #21, which defines the fluid pressure, flowrate, temperature, and physical properties. The fluid inlet conditions are as follows:

Flowrate	67 lb/hr
Temperature	45.0°F
Upstream duct pressure	14.7 psi
Component outlet pressure	14.7 psi

The pump is simulated only to an extent that heat is added to the fluid stream. The amount of heat added is assumed to be 10% of the electrical input power (20 watts). The condensate reservoir is simulated by subroutine TANKG. The required input data is as follows:

Ambient gas temperature	70°F
Conductance between insulation surface & ambient gas	5. Btu/hr-°F
Ambient wall temperature	60
Thermal radiation FA factor	6.0 Ft^2
Structure temperature	60
Conductance between tank wall and structure	5.0 Btu/hr-°F
Conductance between tank wall and outer surface	.5 Btu/hr-°F
Thermal capacitance and tank shell	2.5 Btu/°F
Maximum allowable temp change per iteration	7°F

11. As mentioned in the previous subsection, the rate of sublimation is assumed to equal the rate of precipitation. The amount sublimated is supplied to component 10 as special flow No. 1 from dummy component 19. Since components 10 and 6 alternately switch functions, the data input requirements for 10 and 6 are the same. The assumed conditions for the process heating fluid used to provide thermal energy for the sublimation are summarized below:

Flowrate	45 lb/hr
Inlet temperature	-100 °F
Pressure	20. psia

The physical properties for the heating fluid, which is assumed to be gaseous nitrogen, are as follows:

Specific heat	0.239 Btu/lb°F
Molecular weight	28.
Viscosity	0.036 lb/ft-hr
Density	0.16 lb/ft^3
Thermal conductivity	0.007 Btu/hr-ft-°F

Special Notes -

1. When attempting to match predicted CO_2 removal rate with the desired removal rate, the following parameters may be varied to achieve the desired result:
    a. precipitator channel coolant flow rate
    b. process air volumetric flow rate
    c. precipitator channel heat transfer area
    d. regenerative heat exchange heat transfer area

2. When attempting to match predicted results with experimental results for the same unit configuration, the following parameters should be varified:
    a. mass transfer coefficients for precipitation and sublimation process
    b. component characteristic dimensions
    c. heat transfer characteristics

3.0 CONCLUSIONS AND RECOMMENDATIONS

The subroutines prepared should provide adequate representations of the overall mass and energy balances for the parametric performance of the concepts considered. In preparing the subroutines several areas where additional effort may be warranted are as follows:

- Determining parametric scaling laws for weight, volume, and power for the ten concepts.
- Performing laboratory testing of the concepts to fully define subsystem parameters or physical properties.
- Performing system integration studies for the concepts when coupled with various oxygen regeneration subsystems or complete EC/LS systems.
- Determining the optimum concept by evaluating the parametric performance of each concept for a wide range of mission, environmental, or operating conditions.
- Performing reliability and cost analysis studies for the ten concepts.

The above recommendations cover a wide gambit of effort. It is probable that some of the concepts may be eliminated from further consideration and that the major emphasis should be placed on perhaps 4 or 5 of the concepts.

In selecting the optimum subsystem, certain other intangibles must be considered. For instance, the year in which space type hardware could be expected to be available. Problems with contamination, corrosion, impacts on the cabin thermal environment, and safety must be assessed. Also the subsystems compatibility with the spacecraft power system.

In general it can be stated that concurrently with laboratory testing of the concepts, the computer subroutines should be used to model the test conditions. In addition to providing a test of the adequacy of the computer math models, this will allow a better understanding of the test results. It can also be stated that having defined those system parameters which are important to the mathematical models, additional laboratory testing is necessary to verify the values of these parameters. Several specific areas where improvements could be made in the simulation models are presented in the following subsections.

3.1 Steam Desorbed Resins

Additional laboratory testing is necessary to determine CO_2 and H_2O equilibrium data at temperatures between 180-220°F. This is the temperature range in which CO_2 is desorbed by steam stripping. The data is required since the rate of mass transfer from the bed to gas is equal to the mass transfer coefficient times the difference between the gas phase partial pressure and the equilibrium partial pressure corresponding to the sorbate bed loading. CO_2 equilibrium data is required for CO_2 bed loadings from 0 to 3.5% and H_2O bed loadings from 0 to 40%. H_2O equilibrium data, which is assumed to be independent of CO_2 loading, is required for H_2O bed loadings from 0 to 40%. An empirical correlation for overall mass transfer coefficient as a function of operating conditions is also required. Parametric computer runs then should be made to compare subroutine results with test data. The relative importance of interparticle diffusion needs to be assessed. More important, the mechanism for mass transfer should be carefully re-evaluated. Can the mass transfer rate be predicted strictly from the equilibrium data and mass transfer coefficient, or are the effects of chemical reaction kinetics more important? Should the water vapor transfer be calculated on as stoichiometric basis from the amount of CO_2 desorbed?

Additional testing may be warranted to verify the heats of sorption for CO_2 and H_2O on the resin particles. Physical properties for the particles, such as bulk density, void fraction, superficial surface area, specific heat, etc., must be carefully defined. Additional testing also is required for determining the heat transfer characteristics of the bed. In particular, the effective thermal conductivity of the resin material is required. If the bed contains an integral heat exchanger, the overall thermal conductivity between the heat exchanger/gas or heat exchanger/pellets should be evaluated.

3.2 Vacuum Desorbed Resins

At the present time no equilibrium data is available for Gat-O-Sorb resin which is considered the most promising resin for this concept. Equilibrium data is required for approximately the same set of temperature and bed loadings as for the steam desorbed concept. Data on the physical properties of the resin such as bulk density, superficial surface area, void fraction, etc., also are lacking.

The same general comment made for the steam desorbed resin which called for additional analysis of the mechanism for mass transfer also applies. Additional data also is required for mass transfer coefficients, heat of sorption, and heat transfer characteristics. Since, for this concept, the bed contains an integral heat exchanger, the importance of a careful definition of the heat transfer characteristics should be emphasized.

3.3 Carbonation Cell

The math models for the subroutines used in simulating this concept are relatively unsophisticated. However, additional complexity is most likely not warranted since the concept is generally considered to have been superseded by the hydrogen depolarized cell. Assuming the math models to be adequate, a better definition of cell design characteristics is required for an adequate simulation of the concept. The heat transfer characteristics of a typical cell should be determined. All parameters such as current density and voltage should be correlated as a function of subsystem variables.

Should more sophistication in the math models be desired, an example of where improvements could be made is in the technique for establishing the water transfer rate to the exit streams. Currently the rate is established by fixed input data for relative humidity in the exit streams. A more realistic model could be developed based on the actual transport phenomena occurring. The math model for predicting water transport rates in the component for humidifying process gas prior to entering the cells also is an example where improvement might be warranted.

3.4 Hydrogen Depolarized Cell

The mathematical model for this subroutine was prepared by Hamilton Standard in conjunction with subsystems development studies for the SSP program. As such the routine should provide a good representation of the subsystem.

3.5 Solid Electrolyte Cell

A good comparison between subroutine results with test data was obtained for this subsystem. This was possible to a great extent because of the advanced state of development of the concept. Good documentation of subsystem test results also was available (Reference 5.13).

It should be noted that the mathematical model for the solid electrolyte cells is somewhat empirical in nature. That is, the model relies heavily on the experimental data. Overall current efficiency, H_2 or CO current efficiency, cell voltage (or voltage efficiency) are a few of the parameters which are based on experimental results. While theoretical relationships could be developed, they would not be as accurate as the empirical data. In order to insure accurate computer results over a wide range of operating conditions, additional laboratory testing is required to determine correlations for these critical parameters as a function of operating variables.

A more detailed mathematical model for the carbon deposition reactor could be developed by treating the reactor as a classical tubular reactor. Additional experimentation would be required to determine the effects of reactor geometry and catalyzing effects on the kinetics of the reaction. In particular, the catalyzing effects of the reactor steel wall and water vapor in the inlet stream would have to be incorporated into the rate equations. Alternatively correlations could be developed for CO and H_2 conversion efficiencies as a function of operating variables.

3.6 Liquid Absorption

The mathematical models prepared for the simulation of this concept should be adequate for gross system analysis. More complex models are not warranted at this time since the concept is only in a conceptual stage of development. Many problems remain to be solved in designing zero-g hardware.

When the design concept becomes better defined, there are several areas where improvements could be made in the mathematical models. For the liquid contactor, a subroutine could be prepared with a multiple number of bed elements. Transient macroscopic mass and energy balances could be set-up taking into account mass transfer resistances in both the liquid and gas phases.

Another subroutine which might warrant future development would be an air/liquid separator routine. The subroutine would be modeled after zero-g separator devices currently in the state of development. The separation achieved would be predicted from constituent equilibrium relationships and efficiency factors.

The subroutine for the separation of CO_2 from the liquid phase has been modeled as an equilibrium or flash vaporization process. When the design of this device is better defined, the subroutine could be modified to better reflect the operating characteristics of the device.

It is suggested that system analysis studies be performed leading to the development of a space hardware prototype for this subsystem. Improvements to the existing subroutines could be made concurrently with the prototype development.

3.7 Electrodialysis Cells

The subroutine prepared for this concept should provide an adequate simulation of the "E" stack cell configuration described in reference 7.1. For this configuration a considerable amount of oxygen is generated along with the removal of CO_2. One possible improvement in the routine might be to provide an option for simulating the "F" configuration, which minimizes O_2 production.

The subroutine prepared relies on experimental data for stack voltage, power and current efficiencies. It is suggested that correlations be developed for these parameters as a function of operating variables.

A more sophisticated method for determining the amount of water lost by electro-endosmosis probably is warranted. The current method is based on fixed input values for the humidities in the exit streams. A model based on the physical chemistry of the actual phenomena could be developed and incorporated into the subroutine.

3.8 Molten Carbonate Cells

The subroutine prepared should allow good simulation of molten carbonate cells in which the process air has been pre-dried to prevent water vapor electrolysis and subsequent adverse side reactions. Should future subsystem studies indicate the advisability of developing a cell for combined CO_2 removal and H_2 electrolysis, additional logic would have to be incorporated to simulate the side reactions.

The current subroutine relies on experimental values for power efficiency. Current efficiency is assumed to be 100%. Correlations should be developed for these parameters over a range of operating conditions. While current efficiency should approach 100% for the expected operating conditions, excessive current densities will cause degraded performance.

3.9 Membrane Diffusion

The mathematical model prepared for the diffusion separator should allow a good simulation of this concept. In addition, the subroutine can be used to simulate similar diffusion processes in other subsystems.

The most important parameters, which must be accurately defined, are the permeabilities of the diffusing species. Correlations for permeabilities as a function of system variables should be determined by additional laboratory testing.

3.10 Mechanical Freezeout

No new component subroutines were prepared in order to simulate this concept. A modified version of the heat exchanger subroutine was used to simulate the precipitator and sublimator. The partial pressure of CO_2 leaving the precipitator is predicted from the equilibrium sublimation curve for CO_2 and Dalton's law. Mass transfer rates are not considered. The rate of CO_2 leaving the sublimator is assumed to equal the rate of precipitation. The heat exchanger subroutine calculates the required outlet temperature for the heating fluid necessary to provide the heat of sublimation.

The technique for simulating the precipitation process should provide an adequate simulation. The transient simulation of this process could be improved by preparing a multi-element model with the rate of mass transfer calculated from an overall mass transfer coefficient and the difference between the gas phase partial pressure and the CO_2 equilibrium partial pressure.

The improvements suggested above are even more important for an adequate transient simulation of the sublimator. In order to develop such a model, the design geometry of the precipitator/sublimators must be fully defined. In addition, experimental testing would be required to determine a correlation for mass transfer coefficients as a function of system parameters.

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APPENDIX A

NEW COMPONENT SUBROUTINES

CARDP

Component Subroutine No. 50 - Carbon Deposition Reactor

1.0 Subroutine Description

The carbon deposition reactor, which is also referred to as a carbon disproportionator, reduces CO to carbon. The reactor is a major component of the solid electrolyte subsystem for regenerating O_2 from CO_2 generated in a spacecraft environment. The reactor converts CO generated in the solid electrolyte cells into CO_2 and carbon. The carbon is deposited on the walls of the reactor while CO_2 is recycled to the solid electrolyte cells.

The following two principal reactions occur in the reactor:

$$2\ CO \rightarrow CO_2 + C \tag{1}$$

$$H_2 + CO_2 \rightarrow H_2O + CO \tag{2}$$

The second reaction converts hydrogen into water which, in small amounts, catalyzes both CO_2 decomposition in the electrolyzer and carbon monoxide disproportionation in the reactor. The level of hydrogen in the feed is prevented from building up too high by separating out most of the hydrogen prior to entering the reactor. The separation is performed in a semi-permeable membrane separation device. The degree of separation is controlled by regulating the pressure on the vacuum side of the membrane.

Basically, the reactor is a tubular flow reactor with walls constructed of low carbon steel. The steel serves to catalyze the reaction. The reactor has an internal scrapper for removing carbon deposited on the reactor walls. A jar is located at the bottom of the reactor to collect carbon scrapped from the walls. Alternatively, a disposable reactor tube concept could be used.

The reactor operating temperature is in the range of $550^{\circ}C$. The reactor contains a heater element to bring the reactor up to temperature. Since the reactor is exothermic, the heater is not required during quasi-steady state operation if adequate insulation is provided.

2.0 Subroutine Data

2.1 General Notes

1. A primary source of flow must be specified to provide an inlet gas flow. The primary side flow code must be 3. The flow constituents in the source of flow must be compatible with those for the component.

2. The gaseous feed for the primary side of the component is assumed to be composed primarily of CO_2, H_2O, CO, and H_2. H_2 and CO are assumed to enter as special flows 1 and 2, respectively.

2.2 Heat Loss V-Array Data

Reference Location	Description	Data Type
51	Temperature of reactor (^oF)	0
52	Effective thermal conductance from the reactor to surroundings (Btu/hr ^oF)	0
53	Total heat loss from reactor to surroundings (Btu/hr) R(53) = R(56) + R(59) + R(62)	0
54	Ambient gas temperature (^oF)	I(R)
55	Thermal conductance between surface of reactor insulation and ambient gas ($\frac{Btu}{hr - ^oF}$)	I(R)
56	Convective heat loss to ambient gas from reactor (Btu/hr)	0
57	Ambient wall temperature (^oF)	I(R)
58	Reactor thermal radiation FA from surface of insulation to ambient wall (ft^2)	I(R)
59	Radiation heat loss from reactor to ambient wall (Btu/hr)	0
60	Structure temperature (^oF)	I(R)
61	Conductance ($\frac{kA}{\Delta X}$) between reactor and structure	I(R)
62	Conductive heat loss to the structure (Btu/hr)	0
63	Insulation surface temperature (^oF)	0
64	Conductance ($\frac{kA}{\Delta X}$) between module shell and outer surface of insulation	I(0)

2.3 Steady State V-Array Data

Reference Location	Description	Data Type
65	Heat dissipated in a module by electrical heater (Btu/hr)	I(O)
66	Heat generated by net influx of reactants and products and the heat of reaction (Btu/hr)	O
67	CO conversion (fraction)	I(R)
68	H_2 conversion (fraction)	I(R)
69	Previous trial value for PHI (Btu/hr)	O
70	Previous trial value for TMOD (°F)	O
71	Convergence tolerance for calculating cell temperature (percent)	I(R)
72	Deposition rate for carbon on walls of reactor (lb/hr)	O

2.4 Transient V-Array Data

Reference Location	Description	Data Type
R(73)	Total reactor thermal capacitance (Btu/°F)	I(R)
R(74)	Initial temperature at time t(°F)	I(R)

Table 1

CONSTANTS FOR HEAT CAPACITY EQUATIONS

$$C_p = a/T^2 + b/T + c + dT^1 + eT^2 \quad \frac{\text{cal}}{\text{g mole } ^\circ\text{K}}$$

	a	b	c	d	e
$O_2(g)$	-187700.	0.	8.27	.000258	0.
$H_2O(g)$	0.	0.	8.22	.00015	.00000134
CO_2	-195500.	0.	10.34	.00274	0.
C(graphite)	0.	0.	2.673	.002617	-116900.
H_2	0.	0.	6.62	.00081	0.
CO	0.	0.	6.60	.00120	0.

3.0 Analytical Model Description

The equilibrium constant for the conversion of CO to CO_2 (equation 1) is equal to 36×10^6 at 850°C. Thus from an equilibrium standpoint, the formation of CO_2 is strongly favored. The reaction would be expected to go essentially to completion. The actual conversion, however, may be considerably less due to the kinetics of the reaction.

From a reactor design standpoint, the reactor could be treated as a classical tubular reactor. Standard techniques are available for analysis of a specified design configuration (reference (1)). The reaction rate constant will be influenced by two catalyzing factors: the low carbon steel walls of the container, and the amount of water vapor present in the reactor. Thus as carbon is deposited on the walls of the reactor, the reaction rate will be effected. Fluctuations in the levels of hydrogen in the feed, which reacts to form water, will also influence the reaction rate.

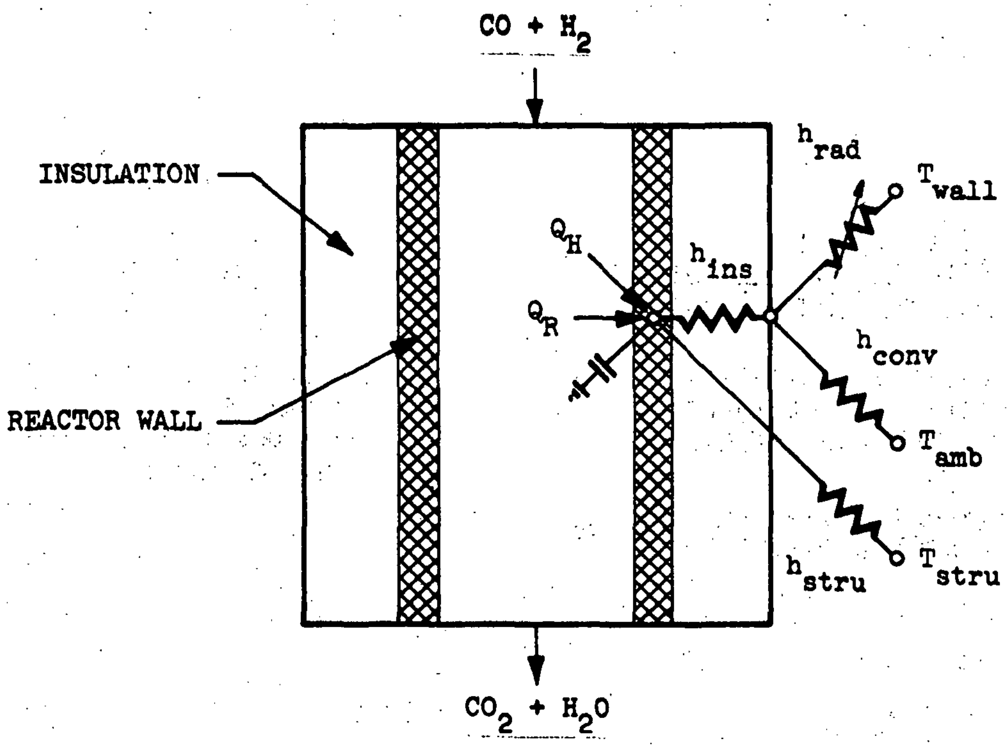
The actual conversion will be difficult to predict analytically since the geometry of the reactor is not fully defined and because of the complex nature of the reaction rate. Thus an empirical approach will be used based on experimentally determined values for CO and H_2O conversion. Thus

$$M_{CO,o} = M_{CO,i} (1-n_1) \tag{3}$$

$$M_{H_{2,o}} = M_{H_{2,i}} (1-n_2) \tag{4}$$

The reactor is treated as a single lumped mass for heat transfer analysis. A heat balance is performed taking into account losses to the ambient due to conduction, radiation, and convection; electrical heater power dissipations; the net enthalpy change of products and reactants; and the heat of reaction. Figure 1 illustrates the thermal model used in the subroutine.

The net enthalpy added by the influx and efflux of reactants and products respectively and the heat of chemical reaction is as follows:



Q_H = HEAT DISSIPATED BY ELECTRICAL HEATER (BTU/HR)

Q_R = ENTHALPY CHANGE FOR NET INFLUX OF REACTANTS AND PRODUCTS AND CHEMICAL REACTION (BTU/HR)

h_{rad} = RADIATION CONDUCTANCE FROM SURFACE OF INSULATION TO AMBIENT WALL (BTU/HR °F)

h_{conv} = CONVECTION CONDUCTANCE FROM SURFACE OF INSULATION TO AMBIENT WALL (BTU/HR °F)

h_{stru} = CONDUCTANCE FROM REACTOR TO STRUCTURE (BTU/HR °F)

FIGURE 1 CROSS SECTIONAL VIEW OF REACTOR TUBE SHOWING THERMAL MODEL

$$\Delta H_T = \Delta H_R - \Delta H_R - \Delta H_{1,To} - \Delta H_{2,To} \qquad (5)$$

where:

ΔH_R = enthalpy change of reactants (Btu/°F)

ΔH_P = enthalpy change of products (Btu/°F)

$\Delta H_{1,T_o}$ = heat of reaction (heat absorbed) for decomposition of CO (Btu/hr)

$\Delta H_{2,T_o}$ = heat of reaction (heat absorbed) for decomposition of H_2 (Btu/hr)

ΔH_R and ΔH_P are the integrated enthalpy changes for the reactants and products, respectively, from the inlet and outlet temperature to the standard state for the heat of reaction (77°F). The integrated enthalpy change for each species is calculated by the following equation:

$$\Delta H_i = N_i \int_{T_o}^{T} (aT^{-2} + bT^{-1} + cT^{o} + dT^{1} + eT^{2})dT \qquad (6)$$

where:

N_i = flow rate of species i (lb/hr)

ΔH_i = enthalpy change for constituent i between temperature T and T_o (Btu/hr)

a, b, c, d = experimentally determined coefficients for heat capacity as a function of temperature. The values of these constants for the reactant and product constituents are given in Table 1.

The net heat balance for the reactor temperature is given below:

$$\frac{T_{RX}' - T_{RX}}{\Delta t} G = -Q_{AM} + Q_e + Q_H \tag{7}$$

when:

Q_{AM} = net heat loss to the surroundings by conduction, convection, and radiation (Btu/hr)

Q_e = electrical energy dissipated by the heater (Btu/hr)

Q_H = net enthalpy added to module by reactants and products (Btu/hr)

T_{RX}', T_{RX} = temperature of reactor at time t + Δt and time t

G = thermal capacitance of reactor (Btu/$^{\circ}$F)

Equation (7) is rewritten in the following form for solution by a trial and error procedure

$$\mathrm{PHI} = - \frac{T_{RX}' - T_{RX}}{\Delta t} G - Q_{AM} + Q_C + Q_H \tag{8}$$

For a trial value of T_{RX}', Q_{AM} is calculated using subroutine QSURR. Equation (8) is solved for PHI. Subroutine ESTDM is then used to determine the value of T_{RX}' for which PHI equals 0. Convergence is satisfied when:

$$\left| \frac{\mathrm{PHI}}{(\Delta H_R + Q_e)} \right| < \frac{R(80)}{100.} \tag{9}$$

4.0 Lower Level Subroutines and Functions

QSURR
ESTIM

5.0 References

J. Smith, "Chemical Engineering Kinetics," McGraw-Hill Book Co., Inc., New York, 1956, p. 96.

C0S0RP

Component Subroutine No. 36 - Two Constituent Sorption Bed Subroutine

1.0 Subroutine Description

This subroutine may be used to simulate the absorption (or adsorption) and desorption of either CO_2 and H_2O or both in a packed resin bed. While the routine was prepared expecially for simulation of an IR-45 solid amine resin bed for absorbing CO_2 from a spacecraft environment, the routine is equally suitable for other sorption beds such as silica gel for adsorbing water vapor or molecular sieves for adsorbing CO_2. Both transient or steady-state performance may be simulated. Logic is also incorporated to simulate purge, steam and thermal/vacuum desorption.

The logic for simulation of the pseudo-steady state performance of the bed is rather unsophisticated compared to that for the transient simulation. For steady state purge absorption or desorption, bed performance is calculated from either an average removal efficiency or an average value of bed loading. Steady state steam desorption calculations consist chiefly of determining the amount of steam required to desorb a bed with a specified CO_2 loading.

Three routines are used in the transient simulation. One was prepared for simulating absorption and purge desorption. The second reutine was prepared for simulating steam desorption. Here the bed is purged with steam until CO_2 is driven off in a chromatographic fashion. The mass flow rate is not constant throughout the bed for this process and thus different coding was required. The third routine is for thermal/vacuum desorption.

Transient performance in the bed is performed by splitting the bed into as many as 24 elements in the direction of flow. Lumped parameter equations are incorporated for gas, bed, and heat exchanger (if any), and the canister wall for each element within the bed.

Heat and mass transfer rates within beds are calculated from built in equations or may be entered as data by the program user. The mass transfer rate is an overall rate and should include the effects of convective mass transfer or diffusion, absorption or desorption reaction rates, and intraparticle diffusion. The mass transfer processes for both CO_2 and H_2O are assumed to occur independent of each other. Equilibrium H_2O vapor pressure over the bed is assumed to be independent of CO_2 bed loading. The CO_2 equilibrium partial pressure is assumed to vary both with CO_2 and H_2O bed loading. Equilibrium relationships have been built into the program for CO_2 and H_2O over IR-45 solid amine beds. Alternatively, isotherm data may be entered in tabular form by the program user.

The subroutine described herein is used to simulate only one component of a CO_2 or H_2O removal or collection system: the sorption bed. Other components such as heat exchangers, control valves, fans, boilers, etc. must be simulated by other appropriate G-189 subroutines. The logic for tying the whole system together, including that for simulating the cyclical operation of the beds, must be incorporated into GPOLY coding or another special purpose subroutine.

2.0 Subroutine Data

2.1 General Notes

1. A primary source flow must be specified to provide an inlet gas flow.
2. If the sorption bed has an integral heat exchanger (NSTR(2) = 1 or 2), a secondary source flow must be specified to provide an inlet liquid flow for heating or cooling.
3. The primary side flow code must be 2 or 3. If there is a secondary flow, its code must be 0 or 4.
4. The flow constituents in the source of flow must be compatible with those for the component.
5. Equilibrium relationships for CO_2 and H_2O partial pressure in solid amine (IR-45) absorption beds have been built into the program. The program user may enter alternate data as table data. The table numbers to be used are then specified in steady state K array reference locations 17, 18, 19, 20.
6. Either single constituent or two constituent sorption processes may be simulated (see NSTR(1)).

7. Isothermal bed calculations may be performed without specifying a heating or cooling fluid by setting NSTR(9) = 1
8. Mass transfer calculations may be bypassed if only heat transfer calculations are desired. (NSTR(10)=1)
9. When simulating thermal/vacuum desorption with the beds switching periodically from an adsorption to a desorption mode, the number of bed elements specified in K(NK+21) should be set equal to the number of bed elements to be used during the absorption mode. During the desorption mode, the routine automatically assumes one bed element.
10. When using the integral heat exchanger option, data should be entered for each of the quantities in R(87) through R(94). Where the effects of these individual quantities are negligible, a small number of the order of 1.0×10^{-12} should be entered as data. This will prevent computational problems in the steady state heat balance.

2.2 Instruction Options

NSTR(1)	Specifies sorbing constituents
= 0	Sorption of CO_2 only
= 1	Sorption of H_2O only
= 2	Co-sorption of CO_2, H_2O
= 3	Co-sorption of CO_2, H_2O. During desorption, the moles H_2O desorbed are assumed to equal moles CO_2 desorbed. The CO_2 desorbed is calculated in the same manner as with NSTR(1) = 0 or 3.

NSTR(2)	Integral heat exchanger for cooling or heating
= 0	Bed has no heat exchanger
= 1	Bed has counter flow heat exchanger
= 2	Bed has parallel flow heat exchanger

NSTR(3)	Specifies method used during desorption
= 1	Steam stripping
= 2	Purge gas
= 3	Vacuum Desorption

NSTR(4)	Heat transfer coefficient between carrier gas and bed during sorption
= 0	Use constant value in R(77)
= 1	Calculate from built-in relationship
NSTR(5)	Mass transfer coefficient between carrier gas and bed during sorption
= 0	Use constant value entered in R(82) or R(86)
= 1	Calculate from built-in relationship
NSTR(6)	Heat transfer coefficient between gas and bed during desorption
= 0	Use constant value entered in R(78)
= 1	Calculate from built-in relationship
= 2	Assume outlet gas temperature equals bed temperature
NSTR(7)	Mass transfer coefficient between gas and bed during desorption
= 0	Use constant value entered in R(81) or R(85)
= 1	Calculate from built-in relationship
= 2	Assume outlet partial pressure for element equals bed equilibrium pressure for H_2O
= 3	Assume outlet partial pressure for element equals bed equilibrium pressures for CO_2 and H_2O
NSTR(8)	Heat transfer coefficient between gas and heat exchanger core
= 0	Use constant value entered in R(87)
= 1	Assume equal to that between gas and bed
NSTR(9)	Specifies a special option for simulating isothermal bed operation during sorption
= 2	Hold bed temperature to a constant value specified in RX(06)
NSTR(10)	Specifies a special option which allows simulation of heat transfer but omits mass transfer in the bed
= 1	Perform heat transfer calculations only

NSTR(11) Heat transfer coefficient between gas and inside wall of bed canister.

= 0 Use constant value in R(92).

= 1 Assume equal to that between gas and bed.

NSTR(12) Specifies method for performing pseudo-steady state sorption or desorption calculations.

= 0 Use constant value for removal efficiency specified in R(65) or R(66).

= 1 Use average value of bed loading $\frac{\text{lb}_{\text{sorbate}}}{\text{lb}_{\text{dry resin}}}$ in R(65) or R(66).

NSTR(13) Instruction for setting initial conditions during transient run. These include: node CO_2, H_2O, and air exit partial pressures; CO_2 and H_2O bed loading; gas, bed, and heat exchanger temperature.

= 0 Input data must be entered for every node.

= 1 Input data is entered only for first node. Corresponding values for the other nodes are set equal to this data.

= 2 Same as 1 except that the CO_2 concentration varies linearly with distance from the value entered for the first node to zero at the last node.

= 3 Same as 1 except that the H_2O concentration varies linearly with distance from the value entered for the first node to zero at the last node.

= 4 Same as 1 except that both the CO_2 and H_2O concentration varies linearly with distance from the value entered for the first node to zero at the last node.

= 5 Same as 1 except input data for CO_2 and H_2O concentration is entered for every node

2.3 Heat Loss V-Array Data

Reference Location	Description	Data Type
R(51)	Temperature of inside surface of bed canister (°F)	0
R(52)	Not used.	

Reference Location	Description	Data Type
R(53)	Total heat lost from component to environment (Btu/hr)	0
R(54)	Ambient gas temperature (^{o}F)	I(0)
R(55)	UA between ambient gas and insulation surface (Btu/hr-^{o}F)	I(0)
R(56)	Temperature of outside surface of insulation (^{o}F)	0
R(57)	Conductance between inside surface of canister and insulation exterior surface (Btu/hr^{o}F)	I(0)

2.4 Steady State K-Array Data

Reference Location	Description	Data Type
16	Bed operating mode	I(R)
= 0	Bed is sorbing	
= 1	Bed is desorbing	
17	H_2O/Resin Equilibrium Isotherm	I(R)
= -N	Use built in relationship for equilibrium H_2O partial pressure over resin	
= +N	Table number for bivariant curve for H_2O equilibrium partial pressure 1st independent variable = H_2O bed loading $\frac{lb_{sorbate}}{lb_{dry\ resin}}$ 2nd independent variable = Bed temperature (^{o}F) dependent variable = partial pressure (mmHg)	
18	CO_2/Resin Equilibrium Isotherms	I(R)
= -N	Use built in relationship	
= +N	Table number for bivariant curve for CO_2 equilibrium partial pressure for H_2O bed loading specified in R(95) 1st independent variable = CO_2 bed loading $\frac{lb_{surbate}}{lb_{dry\ resin}}$	

Reference Location	Description	Data Type
	2nd independent	
	= Bed temperature (°F)	
	dependent variable	
	= partial pressure (mm Hg)	
19	CO_2/Resin Equilibrium Isotherm	
= -N	Use built-in relationship	I(0)
= +N	Table number for H_2O bed loading specified in R(96)	
= 0	Table no. specified in K(NK+18) is used	
20	CO_2/Resin Equilibrium Isotherm	I(0)
= -N	Use built-in relationship	
= +N	Table number for H_2O bed loading specified in R(97)	
= 0	Table no. specified in K(NK+18) is used	

2.5 Steady State V-Array Data

Reference Location	Description	Data Type	
65	CO_2 removal efficiency $\frac{\text{lb sorbate removed}}{\text{lb sorbate entering}}$ if NSTR(12) = 0 or average value of CO_2 bed loading $\frac{lb_{sorbate}}{lb_{dry\ bed}}$ if NSTR(12) = 1	I(R) if NSTR(1) = 0 or 2	
66	H_2O removal efficiency $\frac{lb_{sorbate\ removed}}{lb_{sorbate\ entering}}$ if NSTR(12) = 0 or average value of H_2O bed loading $\frac{lb_{sorbate}}{lb_{dry\ bed}}$ if NSTR(12) = 1	if NSTR(1) = 1 or 2	
67	Resin particle density (lb/ft^3)	I(R)	*
68	Resin bulk density (lb/ft^3)		
69	Resin pellet effective diameter (ft)	I(R)	
70	Resin void fraction (dimensionless)		
71	Resin superficial surface area (ft^2/ft^3)	I(R)	
72	Sphericity (=1.0 for spherical particles)	I(R)	
73	Channeling factor (= 1.0 for no channeling)	I(R)	
74	Bed inside diameter (ft)	I(0)	*
75	Bed frontal area (ft^2)	I(0)	
76	Bed length (ft)	I(R)	
77	Overall heat transfer coefficient between gas and pellets during sorption ($Btu/hr\text{-}ft^2\text{-}°F$)	if NSTR(4) = 0	
78	Overall heat transfer coefficient between gas and pellets during desorption ($Btu/hr\text{-}ft^2\text{-}°F$)		
79	Heat of sorption for CO_2 (Btu/lb)	I(R) if NSTR(1) = 0 or 2	
80	Binary diffusion coefficient (diffusivity) for CO_2/Air (ft^2/hr)	I(R) if NSTR(5) = 1 and NSTR(1) = 0 or 2	

* Input data required for one of these quantities

Reference Location	Description	Data Type
81	Overall mass transfer coefficient (pellet to gas) for CO_2 during desorption $\left(\frac{\text{lb moles}}{\text{hr-ft}^2\text{-mm Hg}}\right)$	I(R) if NSTR(1) 0 or 2 and NSTR(7) = 0
82	Overall mass transfer coefficient (pellet to gas) for CO_2 during sorption $\left(\frac{\text{lb moles}}{\text{hr-ft}^2\text{-mm Hg}}\right)$	I(R) if NSTR(1) = 0 or 2 and NSTR(5) = 0
83	Heat of sorption for H_2O (Btu/lb)	I(R) if NSTR(1) = 1 or 2
84	Binary diffusion coefficient (diffusivity) for H_2O/Air (ft^2/hr)	I(R) if NSTR(5) = 1 and NSTR(1) = 1 or 2
85	Overall mass transfer coefficient (pellet to gas) for H_2O during desorption $\left(\frac{\text{lb moles}}{\text{hr-ft}^2\text{- mm Hg}}\right)$	I(R) if NSTR(1) = 1 or 2 and NSTR(5) = 0
86	Overall mass transfer coefficient (pellet to gas) for H_2O during sorption $\left(\frac{\text{lb moles}}{\text{hr-ft}^2\text{-mm Hg}}\right)$	I(R) if NSTR(1) = 1 or 2 and NSTR(5) = 0
87	Overall heat transfer coefficient between heat exchanger core and gas $\left(\frac{\text{Btu}}{\text{hr-ft}^2\ {}^\circ\text{F}}\right)$	I(0)
88	Heat transfer area between core and gas (ft^2)	I(0)
89	Overall heat transfer coefficient between core and bed $\left(\frac{\text{Btu}}{\text{hr-ft}^2\ {}^\circ\text{F}}\right)$	I(0)
90	Heat transfer area between core and bed (ft^2)	I(0)
91	Heat transfer area between gas and inside canister wall (ft^2)	I(0)
92	Overall heat transfer coefficient between gas and canister wall $\left(\frac{\text{Btu}}{\text{hr-ft}^2\ {}^\circ\text{F}}\right)$	
93	Heat transfer coefficient between fluid and heat exchanger core $\left(\frac{\text{Btu}}{\text{Hr-ft}^2\ {}^\circ\text{F}}\right)$	I(0)

Reference Location	Description	Data Type
94	Heat transfer area between fluid and heat exchanger core (ft^2)	I(0)
95	Value of H_2O bed loading for 1st bivariant CO_2/resin isotherm $\left(\frac{lb_{H_2O}}{lb_{dry\ resin}}\right)$	I(R) if KR(17)> 0 and NSTR(2) = 1 or 2
96	Value of H_2O bed loading for 2nd bivariant CO_2/resin isotherm $\left(\frac{lb_{H_2O}}{lb_{dry\ resin}}\right)$	I(R) if KR(17)> 0 and NSTR(2) = 1 or 2
97	Value of H_2O bed loading for 3rd bivariant CO_2/resin isotherm $\left(\frac{lb_{H_2O}}{lb_{dry\ resin}}\right)$	I(R) if KR(17)> 0 and NSTR(2) = 1 or 2
98	Average bed temperature (°F)	I(R), 0
99	Duration of desorption cycle (hours)	I(R) if NSTR(3) = 1 or NSTR(3)=3

2.6 Transient K-Array Data

Reference Location	Description	Data Type
21	Number of bed elements	I(R)
22	Bed operating mode = 0, sorbing = 1, desorbing	I(R)
23	Flag to reverse temperature, pressure, bed loading profiles = 0, no = 1, yes	I(0)

2.7 Transient V-Array Data

Reference Location	Description	Data Type
R(100)	Resin pellet specific heat ($\frac{Btu}{lb^{o}F}$)	I(R)
R(101)	Thermal capacitance of heat exchanger core (Btu/^{o}F)	I(0)
R(102)	Thermal capacitance of heating or cooling fluid (Btu/^{o}F)	I(0)
R(103)	Multiplying factor, Θ, for minimum computing interval ($0 < \Theta > 1.0$)	I(R)

2.8 Extra V-Array Data

Extra V array locations must be reserved for storing bed and gas conditions during a transient run. The number of extra locations required equals = 9* number of bed elements. Initial conditions must be entered for the first element. The corresponding conditions for the other elements will be set equal to those of the first element.

Reference Location	Description for N^{th} Element	Data Type
104 + 9(N-1)	N^{th} element CO_2 exit partial pressure (mm Hg)	I(0)
105 + 9(N-1)	N^{th} element CO_2 bed loading $\frac{lb_{sorbate}}{lb_{dry\ resin}}$	I(R)
106 + 9(N-1)	N^{th} element H_2O exit partial pressure (mm Hg)	I(0)
107 + 9(N-1)	N^{th} element H_2O bed loading $\frac{lb_{sorbate}}{lb_{dry\ resin}}$	I(R)
108 + 9(N-1)	N^{th} element gas outlet temperature (°F)	I(0)
109 + 9(N-1)	N^{th} element bed temperature (°F)	I(R)
110 + 9(N-1)	N^{th} element heat exchanger core temperature (°F)	I(0)
111 + 9(N-1)	N^{th} element heating/cooling fluid outlet temperature (°F)	I(0)
112 + 9(N-1)	N^{th} element air exit pressure (mm Hg)	I(0)

3.0 Analytical Model Description

3.1 Steady State Simulation

3.1.1 Absorption or Purge Description

Two simplifed models are available for simulating mass transfer in a bed.

a. Based on average removal efficiency

$$\dot{w}_{i,out} = w_{i,in}\,(1-\eta_i) \qquad (1)$$

where:

$\dot{w}_i$ = flow rate of sorbing constituent (either CO_2, H_2O, or both)

η_i = removal efficiency for constituent i

b. Based on average bed loading

$$\dot{w}_{i,out} = (\dot{w}_{i,in} - \dot{w}_{i,r}) \qquad (2)$$

where:

$\dot{w}_{i,r} = \dot{w}_g \left(\frac{M_i}{M_g P_g}\right)(1 - e^{-\beta'}) \times (P_{i,in} - P_{i,b}^{*})$ = rate of sorption of constituent (lb/hr) (3)

$\dot{w}_g$ = flow rate of carrier gas (lb/hr)

M_i = molecular weight of sorbing constituent (lb/lb mole)

M_g = molecular weight of carrier gas (lb/lb mole)

$P_{i,in}$ = partial pressure of sorbing constituent entering bed (mm Hg)

$\beta' \equiv \dfrac{KA_b M_g P_g}{\dot{w}_g}$

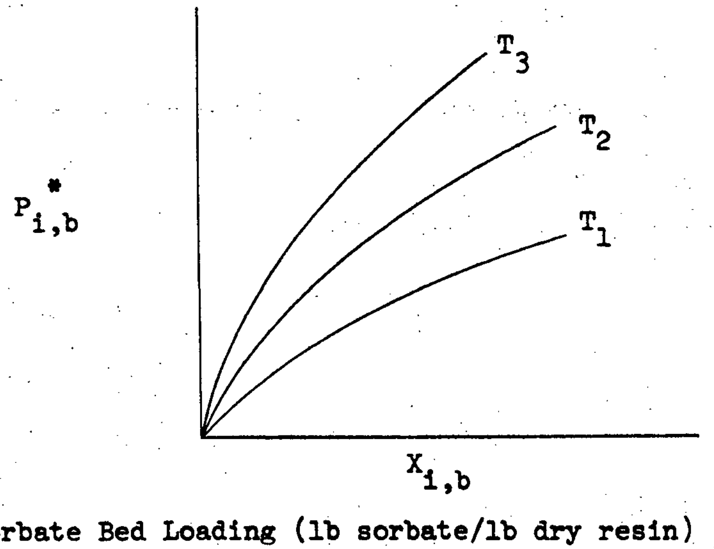
K = mass transfer coefficient between gas and bed (lb moles sorbate/hr-ft^2-mm Hg)

A_b = total surface area for bed material (ft^2)

P_g = total pressure for carrier gas (mm Hg)

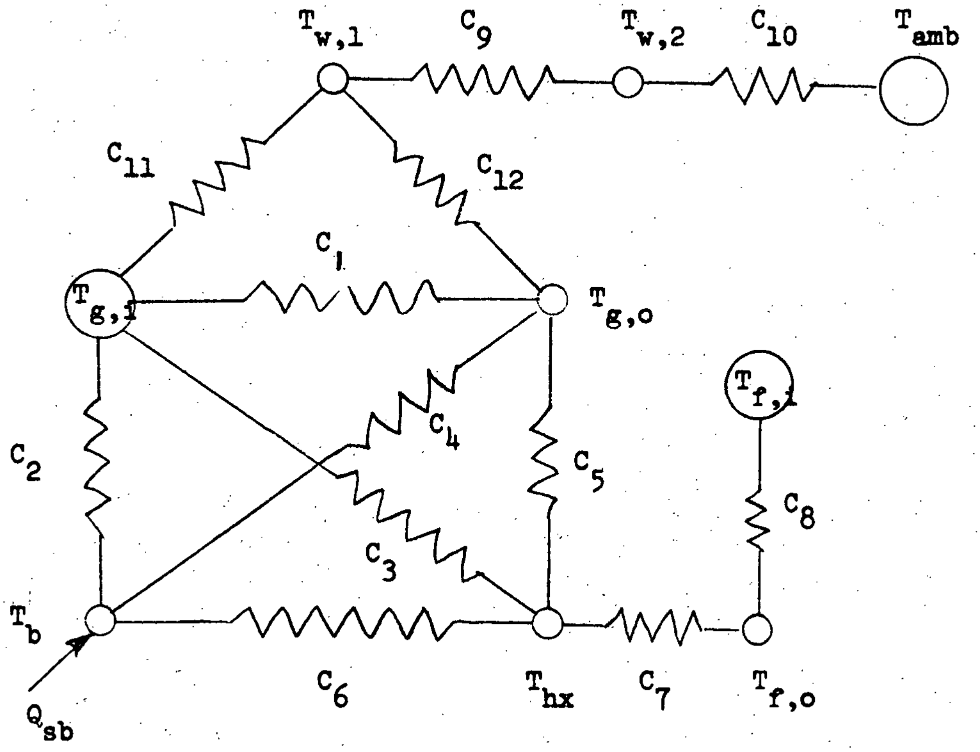
$P_{i,b}^{*}$ = equilibrium partial pressure (mm Hg) for sorbing constituent corresponding to sorbate bed loading (lb sorbate/lb dry resin)

This quantity is conventionally plotted as isotherm curves in the form shown in Figure 1.



Heat transfer in the bed is represented by the thermal analogue shown below:

Figure 2



where:

T_{amb} = ambient temperature (°F)

$T_{w,2}$ = temperature at outside surface of insulation (°F)

$T_{w,1}$ = temperature of inside wall of bed cannister (°F)

$T_{g,i}$ = temperature of process gas entering (°F)

$T_{g,o}$ = temperature of process gas leaving (°F)

T_b = temperature of bed (°F)

T_{hx} = temperature of integral heat exchanger (°F)

$T_{f,i}$ = temperature of heating or cooling fluid entering (°F)

$T_{f,o}$ = temperature of heating or cooling fluid leaving (°F)

where:

$$C_1 = (h_g A_w + h_g A_c + h_g A_b)\left(\frac{1}{1-e^{-\beta}} - \frac{1}{\beta}\right)/(e^{\beta} - 1.)$$

$$C_2 = h_g A_b \left(\frac{1}{\beta} - \frac{e^{-\beta}}{1-e^{-\beta}}\right)$$

$$C_3 = h_g A_c \left(\frac{1}{\beta} - \frac{e^{-\beta}}{1-e^{-\beta}}\right)$$

$$C_4 = h_g A_b \left(\frac{1}{1-e^{-\beta}} - \frac{1}{\beta}\right)$$

$$C_5 = h_g A_c \left(\frac{1}{1-e^{-\beta}} - \frac{1}{\beta}\right)$$

$$C_6 = h_c A_c$$

$$C_7 = h_f A_F$$

$$C_8 = \dot{w}_f C_f$$

$$C_9 = h_I A_I$$

$$C_{10} = h_A A_I$$

$$C_{11} = h_g A_w \left(\frac{1}{\beta} - \frac{e^{-\beta}}{1-e^{-\beta}}\right)$$

$$C_{12} = h_g A_w \left(\frac{1}{1-e^{-\beta}} - \frac{1}{\beta}\right)$$

where:

$h_g A_w$ = thermal conductance between gas and canister wall (Btu/hr-°F)

$h_g A_c$ = thermal conductance between gas and heat exchanger core (Btu/hr-°F)

$h_g A_b$ = thermal conductance between gas and bed (Btu/hr-°F)

$h_I A_I$ = thermal conductance of insulation blanket (Btu/hr-°F)

$h_f A_f$ = thermal conductance between cooling fluid and core (Btu/hr-°F)

$\dot{w}_f C_f$ = flow rate x heat capacity for cooling fluid (Btu/hr-°F)

$h_c A_c$ = thermal conductance between heat exchanger core and bed (Btu/hr-°F)

$h_a A_I$ = thermal conductance between outside surface of insulation and ambient gas (Btu/hr-°F)

Q_{sb} = heat of sorption of constituent (Btu/hr)

For both methods of simulationg steady state performance, the bed is treated as a single element in the direction of flow. The network shown in Figure 2 was transformed into an equivalent thermal analogue which allows solution of the temperatures without iterations.

3.1.2 Steam Desorption

The amount of heat required to desorb a bed with an initial CO_2 bed loading X_s (lb CO_2/lb bed) is given by the following equation:

$$Q = 0.26\ W_p\ (211\ -75.) + 1.\ X_w\ W_p\ (211.\ -75.) + Q_{amb} + X_s\ W_p\ Q_s \qquad (4)$$

where:

Q = total heat required for desorption (Btu/hr)

Q_{amb} = total heat lost by convection and radiation to environment (Btu/hr)

W_p = weight of dry resin in bed (lb)

X_w = average value of water bed loading (lb H_2O/lb dry resin)

X_s = CO_2 bed loading at start of desorption cycle (lb CO_2/lb dry resin)

Q_s = heat of desorption of CO_2 (Btu/lb)

The amount of superheated steam required to provide this heat is given by

$$WSTEAM = Q/L_v \qquad (5)$$

where:

L_v = latent heat of evaporation for steam (Btu/lb)

The CO_2 desorbed is given by the following relationship:

$$R(12) = \frac{X_s W_p}{\tau} \qquad (6)$$

where

τ = duration of desorption cycle (hours)

The amount of water vapor being concurrently desorbed along with the CO_2 is calculated as follows:

$$R(06) = R(12) X (\frac{PW}{PS}) X (\frac{18.}{44.}) \qquad (7)$$

where:

PS and PW equal the equilibrium partial pressures of CO_2 and H_2O, respectively, corresponding to the average value of bed loading X_s, and X_w.

3.1.3 Thermal/Vacuum Desorption

The rate of CO_2 desorption is calculated as follows:

$$R(12) = \frac{X_s W_p}{\tau} \qquad (6)$$

The rate of H_2O desorption is calculated by the following relationship:

$$R(06) = R(12) X (\frac{PW}{PS}) X (\frac{18.}{44.}) \qquad (7)$$

where:

X_s, W_p, τ, PW, and PS previously defined

The total heat required for the desorption process is calculated as follows:

$$A = R(12) \times Q_S + R(06) \times Q_W + Q_{AMB} \qquad (8)$$

where:

Q_W = heat of sorption of H_2O (Btu/lb)

Q_S, Q_{AMB} defined previously

The temperature change for the process heating fluid is as follows:

$$R(21) = B(02) - \frac{Q}{(WC_P)_B} \qquad (9)$$

where:

$(WC_P)_B$ = flow rate x specific heat for heating fluid (Btu/°F)

The outlet pressure for the desorbing gas is assumed to equal to the sum of the equilibrium partial pressure of H_2O and CO_2 corresponding to the average values of bed loading at a bed temperature of 180°F.

3.2 Transient Simulation

3.2.1 Absorption or Purge Desorption

The computer logic for the transient absorption routine is patterned after the mathematical model developed in Reference 1. The same equations described in Section 3.1.1, part b, for the steady state absorption are applied in the transient model. However, the bed is divided into up to 24 elements in the direction of flow.

Heat and mass transfer coefficients between gas and pellets may be entered as data into the program by the program user or built in relationships may be used. For heat transfer the following equations may be used:

for $P_e < 10$

$$\frac{h\,D_p}{k} = \frac{\phi s}{6\,(1-\varepsilon)}\,Pe \qquad (10) \qquad \text{Reference 2}$$

for $P_e > 10$

$$\frac{h\,D_p}{k} = J_H\,C_p\,G\,P_r^{-.666} \qquad (11) \qquad \text{Reference 3}$$

where:

$j_H = 0.61 \, Re^{-.41}$

$Re = \frac{G}{A_v M_f \phi_s \psi}$

h = convective heat transfer coefficient (Btu/hr-ft^2-°F)

D_p = pellet diameter (ft)

k = gas thermal conductivity (Btu-ft/ft^2-hr-°F)

ϕ_s = particle shape factor or sphericity

ε = void fraction

ψ = channeling factor

P_e = Peclet number for heat transfer

C_p = gas heat capacity (Btu/lb-°F)

G = bed mass velocity (lb/ft^2-hr)

P_r = gas Prandtl number

A_v = superficial surface area (ft^2/ft^3)

M_f = gas viscosity (lb/ft-hr)

Analogous equations may be used for the rate of mass transfer. These equations should be used only when experimental data is unavailable. These equations ignore reaction rates and intraparticle diffusion which may be important for certain sorption operations. A technique for "backing out" mass transfer coefficients from experimental "break thru" curves is given in reference 4.

The rate of mass transfer in sorption beds depends on the sorbate equilibrium partial pressure corresponding to the sorbate bed loading. For a solid amine CO_2 absorption bed, co-sorption phenomena must be taken into account since H_2O and CO_2 are simultaneously being absorbed or desorbed during a bed cycle. Thus, for this routine, equations have been built into the routine which allow prediction of the mass transfer for both constituents.

The program has options which allow equilibrium partial pressure isotherm curves to be entered in tabular form as input data. The subroutine also has built in functional relationships which may be used. These relationships apply only to H_2O and CO_2 in equilibrium with IR-45 solid amine resin and are based on a limited amount of experimental data. For H_2O vapor the equilibrium partial pressure has been found to be independent of CO_2 bed loading. Available data has been correlated as follows:

$$P^{*}_{H_2O} = .0996972 + 0.246341\,X_w + 68.7792\,X_w^{2} - 700.607\,X_w^{3} + 262548\,X_w^{4} - 3409.82\,X_w^{5} \qquad (12)$$

and

$$P^{*}_{H_2O,\,T} = P^{SAT}_{H_2O,\,T}\left[\frac{P^{*}_{H_2O,\,77}}{P^{SAT}_{H_2O,\,77}}\right]^{\frac{537}{T}} \qquad (13)$$

where:

$P^{*}_{H_2O,T}$ = equilibrium vapor pressure over IR-45 with water loading X_w at temp. T (psia)

X_w = water bed loading (lb H_2O/lb dry resin)

$P^{*}_{H_2O,77}$ = equilibrium vapor pressure over IR-45 with water loading X_w at temp 77°F

$P^{SAT}_{H_2O,\,T}$ = the saturation pressure of water at temperature T (psia)

For CO_2 the equilibrium partial pressure has been found to depend on the H_2O bed loading as well as CO_2 bed loading:

$$P^{*}_{CO_{2},77} = \left[\frac{0.587}{\ell n\ (.24 + 16.7\ X_w) - \ell n\ (100\ X_s)}\right]^2 \frac{14.7}{760} \qquad (14)$$

and

$$P^{*}_{CO_{2},T} = P^{SAT}_{CO_{2},T} \left[\frac{P_{CO_{2},77}}{P^{SAT}_{CO_{2},77}}\right]^{539/T} \qquad (15)$$

Functions have been built into the program for H_2O and CO_2 saturation pressure as a function of temperature.

The simulation of the heat transfer in the bed is similar to that desired for the steady state module. In the transient model, each element has a thermal analogue similar to Figure 2. Lumped thermal capacitances are included for the bed, heat exchanger, and cooling fluid nodes. Temperatures for these nodes are solved by standard forward difference techniques.

3.2.2 Steam Desorption

In the steam desorption of resins, desorption is accomplished by flowing superheated steam into the bed in the axial direction. The steam condenses on the resin, heats the resin and drives off CO_2. The process occurs in "chromatographic" fashion. The displaced CO_2 is reabsorbed immediately ahead of the steam zone and air is displaced ahead of the CO_2-rich zone.

The computer logic required in this subroutine differs considerably from that for the absorption (or purge desorption) routine because of the "chromatographic" nature of the desorption process. The mass flow rate of the carrier gas (in this case steam) is not constant throughout the bed.

where:

M_i = mass flow of constituents entering element (lb/hr)

i = 1 = CO_2

= 2 = Steam

= 3 = Air

M_i' = mass flow of constituents leaving element (lb/hr)

H_i = enthalpy of constituents entering element (Btu/lb)

H_i' = enthalpy of constituents leaving element (Btu/lb)

$h_w A_w$ = thermal conductance between gas and wall of canister (Btu/hr-°F)

$h_b A_b$ = thermal conductance between gas and bed (Btu-hr-°F)

$h_c A_c$ = thermal conductance between gas and heat exchanger core (Btu/hr-°F)

dm_i = mass of constituent absorbed in element (lb/hr)

$\bar{T} = (T_1 + T_2)/2.$

T_1 = temperature of gas entering element (°F)

T_2 = temperature of gas leaving element (°F)

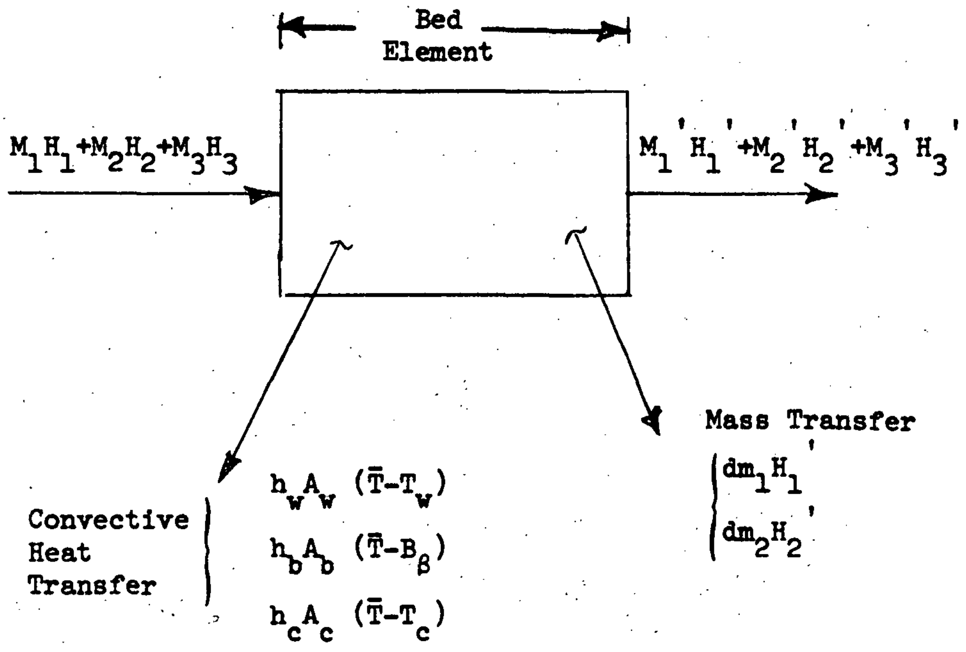
T_w = temperature of canister wall (°F)

T_b = temperature of bed (°F)

T_c = temperature of heat exchanger core (°F)

In order to prevent mathematical and computational difficulties, a small amount of air is introduced along with the steam. This flow is assumed to remain constant throughout the bed. The same equations used for the absorption routine then can be used (equations (2) and (3)) for predicting the mass transfer rates. The following additional assumptions were made in formulating the mathematical model for the routine.

1. The void volume in each element is not considered in the mass transfer equation for each element.
2. Pressure drop in the bed due to friction is neglected.
3. The same relationships used in the absorption routine are used in predicting heat and mass transfer rates and gas equilibrium partial pressures.
4. Gaseous heat transfer is modeled by an enthalpy balance illustrated by Figure 3.



3.2.3 Thermal Vacuum/Desorption

In order to overcome the small allowable stability time computing interval associated with a multi-element model, the desorbing bed is treated as a single element. Since pressure gradients through the bed are relatively small, the single element model is sufficient for most analyses. The same model breakdown for the element is used as was shown in Figure 2. The following additional assumptions were used in preparing the analytical model.

1. Flow rate out of the bed is calculated by the vacuum pump component subroutine. The flow calculated is dependent both on bed pressure and the accumulator pressure into which the desorbing gas is being pumped. Thus, a minimum of at least three component subroutines is required for simulating a desorbing bed: the desorbing bed (CØSØRP), the vacuum pump (VACPMP), and the accumulator (TANKG). In addition, pipe (PIPE) or duct (DUCT) components may be inserted to simulate heat losses to the ambient.

2. The desorbing gas, which consists of a mixture of CO_2 and H_2O, has a pressure equal to the sum of the equilibrium partial pressures corresponding to the bed loadings for CO_2 and H_2O.

3. Mass concentration gradients within the pellet are negligible.

4. The rate of change of bed loading for sorbate i is given by the following relationship.

$$\frac{X_{A,i}' - X_{A,i}}{\Delta\Theta} KV = - Q_Z \, p_{2,i} \tag{16}$$

where:

Q_Z = total volumetric flow rate leaving the bed (ft^3/hr)

$p_{2,i}$ = equilibrium partial pressure of sorbate i

V = total bed volume (ft^3)

$\Delta\theta$ = calculation interval (hours)

$X_{A,i}$ = average bed loading for constituent i at time t $\left(\frac{\text{lb sorbate}}{\text{lb dry resin}}\right)$

$X'_{A,i}$ = average bed loading for constituent i at time t + $\Delta\theta$ $\left(\frac{\text{lb sorbate}}{\text{lb dry resin}}\right)$

$K = (k_i E + (1-E) \frac{\rho i RT}{Mi})$

and

$k_i = \frac{dp}{dx}$ = slope of equilibrium curve for constituent i $\left(\frac{\text{mm Hg}}{\text{lb sorbate/lb dry resin}}\right)$

E = bed void fraction

ρi = particular density (lb/ft^3)

R = universal gas constant = 555. $\frac{(\text{mm Hg})\ (ft^3)}{(\text{lb moles} - {}^{o}R)}$

T = bed temperature (^{o}R)

Mi = molecular weight of sorbate i

5. Pressure drop within the bed for the desorbing gas is calculated by the Blake-Kozeny relationship:

$$\Delta P = \frac{V_o\ 150\mu(1-E)^2 L}{D_P^2\ E^3\ g_c} \qquad (17)$$

where:

V_o = superficial velocity (ft/hr)

ΔP = pressure drop (lb/ft^2)

L = one-half total length of bed (ft)

μ = viscosity of gas mixture (lb/ft-hr)

$$\approx \frac{\Sigma y_i \, \mu_i (M_i)^{1/2}}{\Sigma y_i (M_i)^{1/2}}$$

y_i = mole fraction of sorbate i in gas phase

D_p = particle diameter (ft)

g_i = conversion factor for lb_m to lb_f

= 41.8×10^7 (ft/hr^2) (lb_m/lb_f)

6. The same basic heat transfer model is used for calculating bed temperature as shown in Figure 2. An exception is that the gas temperature is assumed to equal the bed temperature.

4.0 Lower Level Subroutines and Functions

VALUE
PØLYFT
VLH2Ø
VLCØ2
HF
HG
CØABS

SDESRP
SSSØR
VACDSP
VV

5.0 References

1. Blakely, R. L. and Taylor, B. N., "Computer Analysis Techniques for Spacecraft Adsorption Beds," DAC Paper 5159, presented at AIChE Meeting at New Orleans, Louisiana, March 1969.

2. Kunii, D. and Suzuki, M., "Particle-to-Fluid Heat and Mass Transfer in Packed Beds of Fine Particles," International Journal Heat and Mass Transfer, Vol. 10, pages 845-852, 1967.

3. Bird, Stewart, and Lightfoot, "Transport Phenomenon," John Wiley & Sons, Inc., 1960, page 411.

4. Jackson, J. K., "Heat and Mass Transfer Analysis of Adsorption Beds Used in Spacecraft Life Support Systems," Douglas Report SM-47721, 18 September 1964, page 20.

H20SUM

Component Subroutine No. 12 - Water Summation

1.0 Subroutine Description

This subroutine is used to sum up the flows of condensate from 1 to 5 condensing heat exchangers. The subroutine also determines the mix temperature of the condensate flows. The total flow and temperature for the primary side of this component are set equal to these quantities.

2.0 Subroutine Data

2.1 General Notes

1. No source, either primary or secondary, is specified in K(NK+2) or K(NK+5).

2. The number of flows to be summed is entered in K(NK+16). The components which are the sources of condensate are entered in K(NK+17) through K(NK+21). A positive value is entered for the component number if the condensate is from the primary side of the component. A negative value is entered for the component number if from the secondary side.

3. The pressure of the water leaving H20SUM is set equal to the value entered in R(3).

2.2 Steady State K-Array Data

Reference Location	Description	Data Type
16	Number of flows to be summed (1 to 5)	I(R)
17	First component which is a source of condensate flow	I(R)
18	Second component which is a source of condensate flow	I(0)
19	Third component which is a source of condensate flow	I(0)
20	Fourth component which is a source of condensate flow	I(0)
21	Fifth component which is a source of condensate flow	I(0)

3.0 Analytical Model

The total flow and temperature are calculated as follows:

$$R(01) = \sum_{i=1}^{5} \dot{W}_i$$

$$R(02) = \frac{\sum_{i=1}^{5} \dot{W}_i T_i}{R(01)}$$

where:

$\dot{W}_i$ = total flow of condensate from source i

T_i = temperature of condensate flow from source i

4.0 Lower Level Subroutines Required

VV

KK

5.0 References

None.

ELDIAL

Component Subroutine No. 53 - CO_2 Electrodialysis

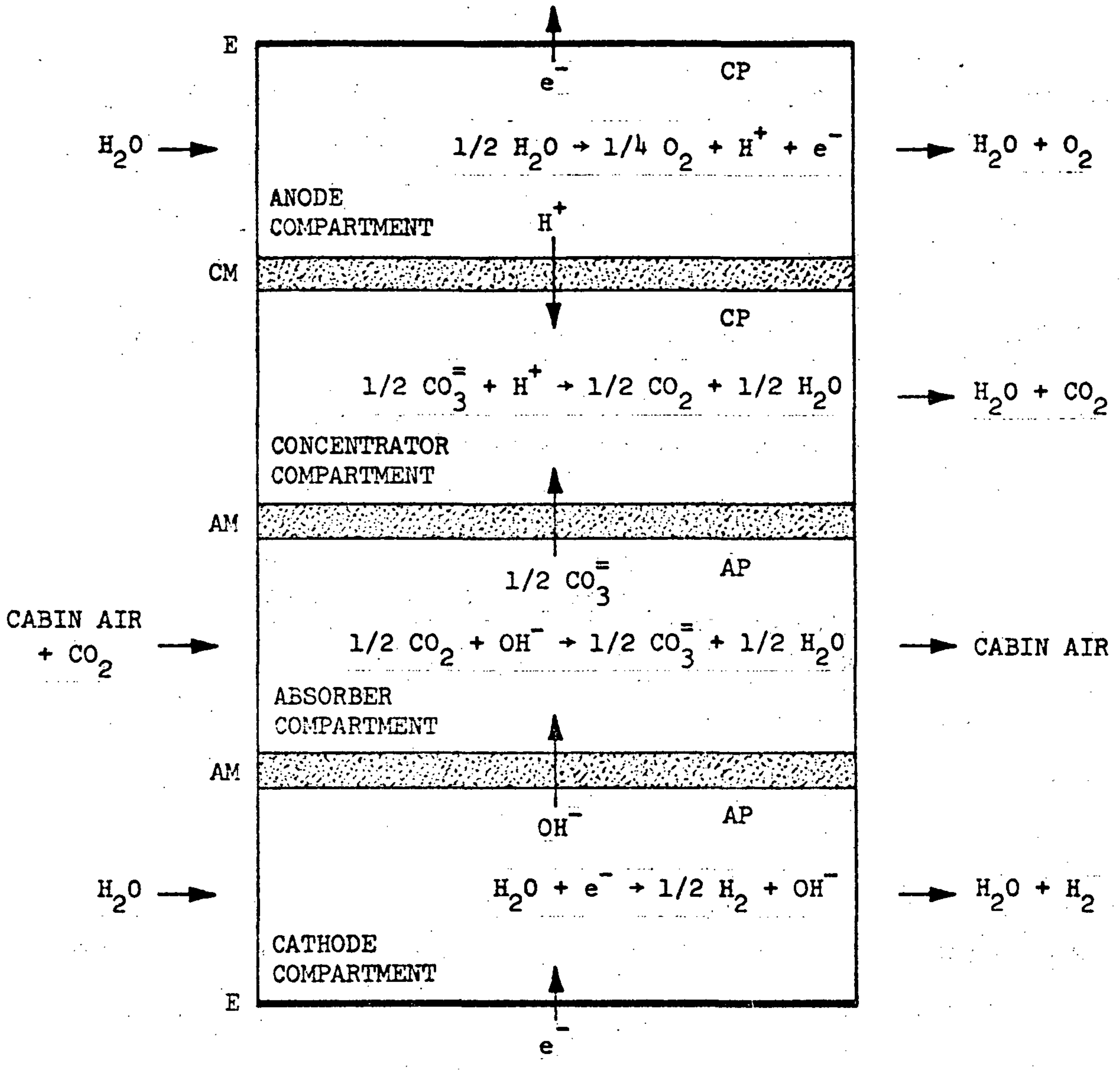
1.0 Subroutine Description

The performance of a CO_2 electrodialysis module may be simualted with this subroutine. In this process, CO_2 is electrochemically separated from cabin air. The CO_2 separated may be stored or sent to an oxygen regeneration subsystem.

The electrodialysis module consists of stacks of repeating cell units of the type illustrated in Figure 1. Cabin air enters the absorber compartment where CO_2 is "scrubbed" out. The absorbed CO_2 is converted to $CO_3^{=}$ by reaction with $\overline{OH}$ ions generated by electrolysis in the cathode compartment of the stack. An anion transfer membrane between these compartments allows the $\overline{OH}$ to permeate into the absorber compartment. Because of the negative charge on the cathode, no $CO_3^{=}$ will permeate into the anode compartment. However, because of the positive charge on the anode, the $CO_3^{=}$ ions will be drawn into the concentrator compartment. Another anion transfer membrane is used here to allow only $CO_3^{=}$ ions to be transferred. In the concentrator compartment, $CO_3^{=}$ reacts with H^+ to reform CO_2. The H^+ ions are generated by electrolysis in the anode compartment of the stack. A cation transfer membrane is employed between the cathode and concentrator compartments to allow transfer of only the H^+ ions. The H^+ ions are caused to migrate because of the negative charge at the cathode.

The above description does not discuss water permeation across the membranes. Water permeation does occur and is referred to as electroendosmosis. Water molecules may be thought of as being dragged along with the migrating ions.

The subroutine prepared considers the electrodialysis module to be comprised of a number of stacks containing a multiple number of cell units of the type shown in Figure 1. The multiple compartments of each stack are assumed to be situated between a single pair of electrodes.



CM	CATION-TRANSFER MEMBRANE
AM	ANION-TRANSFER MEMBRANE
CP	MACROPOROUS CATION-CONDUCTING PACKING
AP	MACROPOROUS ANION-CONDUCTING PACKING
E	BIPOLAR METAL ELECTRODE

FIGURE 1 CARBON DIOXIDE SCRUBBER (SCHEMATIC OF BASIC REPEATING UNIT)

For heat transfer purposes, each cell module is treated as a single lumped mass. Temperature gradients between compartments are ignored.

Because of the complex nature of the electroendosmosis phenomena, water transfer across the membranes will be set by input values for the relative humidity of the exit streams. That is, enough water will be transferred across the membranes to satisfy the relative humidity requirement. Values for relative humidity should be based on experimental results for a typical module.

The subroutine has an option which allows a sweep stream to be used in the concentrator compartment. Either gas or liquid streams may be specified.

2.0 Subroutine Data

2.1 General Notes

1. A primary source of flow must be specified to provide the process gas flow. The primary side flow code must be 2 or 3. The flow constituents in the source of flow must be compatible with those for the component.
2. As a program option, a secondary source of flow may be specified for "sweep" flow to the concentrator compartments. If the sweep flow is liquid, a flow code of 4 must be specified for the secondary side of the component. Special flow No. 2 will be assumed to be the sweep flow, and special flow No. 5 the collected CO_2. If the sweep flow is gaseous, a flow code of 2 or 3 must be specified. The collected CO_2 will be in R(31). If there is no sweep flow, a flow code of 2 or 3 must be specified. The collected CO_2 again will be in R(31).
3. The electrodialysis unit has two additional inlet streams which provide water for electrolysis in the anode and cathode compartments. An "alternate" component must be specified for storing the outlet conditions for these two streams. The primary side for the alternate component is assumed to be the stream leaving the anode compartment of the module. Similarly, the secondary

side for the alternate component is assumed to be the stream leaving the cathode compartment. This alternate component should not be put in the solution path. Figure 2 illustrates the flow streams to the component and alternate component.

4. A flow code of 4 must be specified for the primary side of the alternate component. Using this option, the total flow out will be the sum of special flows 2 through 6. Special flow 2 is assumed to be liquid water. Special flow 3 is assumed to be oxygen generated by electrolysis. Special flows 4 thru 6 equal 0.

5. The flow code for the secondary side of the alternate component also must be 4. Special flow 2 is liquid water and special flow 4 hydrogen. Special flows 3, 5, 6 equal 0.

6. The components which supply sources of flow to the primary and secondary side of the alternate component are assumed to provide pure liquid water.

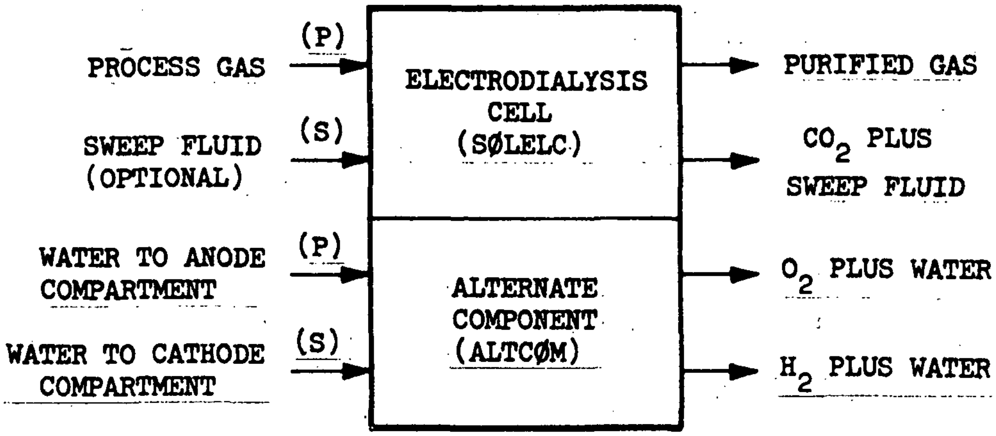
2.2 Instruction Options

NSTR(1): Specifies a sweep fluid for the concentrator compartment.

= 0 no sweep fluid
= 1 sweep fluid is a gas
= 2 sweep fluid is a liquid

NSTR(2): Specifies method for determining current efficiency

= 0 current efficiency is a constant value entered in R(68)
= 1 interpolates table data for current efficiency (fraction) as a function of CO_2 feed rate (lb/hr-ft^2) and current density (amps/ft^2).



IN ALL LIQUID STREAMS:

SPECIAL FLUID 2 = LIQUID WATER
3 = OXYGEN
4 = HYDROGEN
5 = CARBON DIOXIDE

FIGURE 2 FLOW STREAMS TO ELECTRODIALYSIS MODULE

2.3 Heat Loss V-Array Data

Reference Location	Description	Data Type
51	Temperature of module(°F)	0
52	Effective thermal conductance from the module to surroundings (Btu/hr °F)	0
53	Total heat loss from module to surroundings (Btu/hr) R(53) = R(56) + R(59) + R(62)	0
54	*Ambient gas temperature (°F)*	I(R)
55	Thermal conductance between surface of module insulation and ambient gas $(\frac{Btu}{hr\text{-}°F})$	I(R)
56	Convective heat loss to ambient gas from module (Btu/hr)	0
57	Ambient wall temperature (°F)	I(R)
58	Reactor thermal radiation $\mathcal{F}A$ from surface of insulation to ambient wall (ft^2)	I(R)
59	Radiative heat loss from module to ambient wall (Btu/hr)	0
60	Structure temperature (°F)	I(R)
61	Conductance $\frac{kA}{\Delta X}$ between module and structure	I(0)
62	Conductive heat loss to the structure (Btu/hr)	0
63	Insulation surface temperature (°F)	0
64	Conductance $\frac{kA}{\Delta X}$ between module shell and outer surface of insulation	I(0)

2.4 Steady State K-Array Data

Reference Location	Description	Data Type
16	Component number for alternate component	I(R)
17	Number of stacks per module	I(R)
18	Number of absorber/concentrator or anode/cathode compartment cell pairs	I(R)
19	Table number for current efficiency (fraction) as a function of CO_2 feed rate ($lbCO_2/hr\text{-}ft^2$) and current density ($amps/ft^2$)	I(0)

2.5 Steady State V-Array Data

Reference Location	Description	Data Type
65	Net heat generated in module (Btu/hr)	0
66	Current density (amps/ft^2)	I(R)
67	Area per anode (ft^2)	I(R)
68	Current efficiency (based on $CO_3^=$) (fraction)	I(R)
69	Relative humidity of process air stream leaving absorber compartment (percent)	I(R)
70	Relative humidity of sweep gas leaving concentrator compartment (percent)	I(R) if NSTR(1)≠2
71	Stack voltage (volts)	I(R)
72	Power efficiency (fraction)	I(R)
73	Previous trial value for PHI (Btu/hr)*	0
74	Previous trial value for T_{MOD} (°F)*	0
75	Convergence tolerance for calculating cell temperature (percent)	I(R)
76	Water lost by electrolysis (lb/hr)	0
77	Water added to process air by chemical reaction (lb/hr)	0
78	Water added to process air by endosmosis (lb/hr)	0
79	Water added to sweep fluid by chemical reaction (lb/hr)	0
80	Water added to sweep fluid (if a gas) by endosmosis (lb/hr)	0
81	Total water lost by electrolysis, chemical reaction, and endosmosis	0
82	Makeup water required for anode compartment (lb/hr)	0
83	Makeup water required for cathode compartment (lb/hr)	0

2.6 Transient V-Array Data

Reference Location	Description	Data Type
84	Total module thermal capacitance (Btu/°F)	I(R)
85	Initial temperature of module at time t (°F)	I(R)

---

* These quantities are used in the trial and error method used for determining module temperature. The technique is described in Section 3.0.

TABLE 1

CARBON DIOXIDE ABSORBER REACTIONS

Basis: Passage of 1 Faraday of electricity between electrodes = e^-

Component	Reaction Taking Place
Cathode Cell:	$H_2O + e^- \longrightarrow OH^- + 1/2\ H_2$
Anion Transfer Membrane:	$OH^-\ (\text{cathode}) \xrightarrow[\text{ion transport}]{\text{membrane}} OH^-\ (\text{absorber})$
Absorber Cell:	$OH^- + 1/2\ CO_2 \longrightarrow 1/2\ CO_3^{=} + 1/2\ H_2O$
Anion Transfer Membrane:	$1/2\ CO_3^{=}\ (\text{absorber}) \xrightarrow[\text{ion transport}]{\text{membrane}} 1/2\ CO_3^{=}\ (\text{concentrator})$
Concentrator Cell:	$H^+ + 1/2\ CO_3^{=} \longrightarrow 1/2\ CO_2 + 1/2\ H_2O$
Cation Transfer Membrane:	$H^+\ (\text{concentrator}) \xleftarrow[\text{ion transport}]{\text{Membrane}} H^+\ (\text{anode})$
Anode Cell:	$1/2\ H_2O \longrightarrow H^+ + 1/4\ O_2 + e^-$

- -

Overall Reactions:	$1/2\ CO_2\ (\text{absorber}) \longrightarrow 1/2\ CO_2\ (\text{concentrator})$
	$e^-\ (\text{anode}) \xrightarrow[\text{circuit}]{\text{external}} e^-\ (\text{cathode})$
	$1/2\ H_2O\ (\text{electrodes}) \longrightarrow 1/2\ H_2\ (\text{cathode})$ $+ 1/4\ O_2\ (\text{anode})$
	$H_2O\ (\text{electrodes}) \longrightarrow 1/2\ H_2O\ (\text{absorber})$ $+ 1/2\ H_2O\ (\text{concentrator})$

3.0 Analytical Model Description

Table 1 illustrates the chemical and electrochemical reactions occurring in a CO_2 electrodialysis module of the type shown schematically in Figure 1. While Figure 1 shows only a single unit of absorber/concentrator and anode/cathode compartment cell pairs, the discussion which follows applies to any arbitrary number of repeating units.

CO_2 is converted to $CO_3^{=}$ ions in the absorption compartments by reaction with $\overline{OH}$ ions. The $CO_3^{=}$ ions react with H^+ ions in the concentrator compartments to reform CO_2. For the type of electrodialysis cell simulated in this routine, all of the H^+ and $\overline{OH}$ involved in these reactions are formed as the result of electrolysis reactions in the anode and cathode compartments. Thus, the CO_2 removed in the cells can be calculated from the amount of water electrolyzed. The amount of water electrolyzed can be determined by Faraday's law.

$$\dot{m}_{H_2O} = \frac{N}{(96{,}500)(2)} \quad \frac{\text{g moles } H_2O}{\text{amp-sec}} \tag{1}$$

From the equations shown in Table 1, one g mole of CO_2 will be absorbed for every g mole H_2O alectrolyzed. Thus,

$$g = \frac{Q\Delta C}{100\ aN} = \frac{31\ i\ e}{Z} \quad \frac{\text{ft}^2\text{/hr } CO_2 \text{ absorbed}}{\text{ft}^2 \text{ of transfer area}} \tag{2}$$

where:

Q = volumetric flow rate of air flowing through the module (ft^3/hr)
C = concentration of CO_2 in air stream, vol %
a = transfer area per anode (ft^2/cell)
N = total number of pairs of absorber/concentrator or anode/cathode compartments
i = applied current density ($amps/ft^2$)
e = current efficiency (percent)
$= 96{,}500 \frac{\text{amp-sec}}{\text{g - equivalent}}$
Z = g - equivalents/g mole CO_2

The equations shown in Table 1 indicated that for every 1/2 mole H_2O electrolyzed an additional mole of H_2O is lost by migration of H^+ and $\overline{OH}$ ions to the concentrator and absorber compartments. In addition to this amount, water is lost by the phenomena of electroendosmosis. The rate of transfer of water by this mechanism is determined by inputing values for the relative humidity of the streams leaving the absorber/concentrator compartments. This sets the amount of water in the exit streams. The amounts of water formed by electrochemical reactions in these compartments can be calculated by the stoichiometry of the reactions. Thus, the amount of water transferred by electroendosmosis is calculated by the net difference between the water leaving and entering the compartment and water formed by chemical reaction.

For transient heat transfer calculations, the module is treated as a single lumped mass. Thus, the exit streams for each of the four compartments are all assumed to be at one temperature. A heat balance is performed taking into account losses to the ambient due to conduction, radiation, and convection; heat absorbed by the electrolysis reaction and inefficiency in the electrochemical reactions; and the net enthalpy change for the reactants and products. Figure 2 illustrates the thermal module used for this subroutine.

The transient heat balance used on a module is given below:

$$\frac{T_{MOD}' - T_{MOD}}{\Delta\theta} G = -Q_{AM} + Q_e + \Sigma(m\bar{C}_P)_R(T_i - T_R)$$
$$-\Sigma(m\bar{C}_P)_P(T_o - T_R) - \Delta H_R \qquad (3)$$

where:

Q_{AM} = heat lost from module to ambient by radiation, convection and convection (Btu/hr)

Q_e = heat generated in module by inefficiency in electrochemical conversion process (Btu/hr)

$\Sigma(m\bar{C}_P)_R\ T_i$ = enthalpy of reactants entering module Btu/hr)

$\Sigma(m\bar{C}_P)_P\ T_o$ = enthalpy of products leaving module (Btu/hr)

ΔH_R = heat of reaction (heat absorbed) for electrolysis of water at standard state of 25°C (Btu/hr)

G = module thermal capacitance (Btu/°F)

$\Delta\Theta$ = time interval (hours)

T_{MOD}', T_{MOD} = temperature of module at time $t + \Delta\Theta$ and time t, respectively (°F)

T_R = temperature at standard state, 25°C (77°F)

The amount of heat generated in the module by inefficiency in the electrochemical conversion process is calculated as follows:

$$Q_e = IE\ (1-\eta) \times 3.41 \tag{4}$$

where:

I = total current passing through module (amps)

E = total stack voltage (volts)

η = power efficiency (fraction)

The heat balance shown in equation (3) is solved by a trial and error iteration procedure. In this procedure (3) is re-written as follows:

$$PHI = -\frac{T_{MOD}' - T_{MOD}}{\Delta\Theta} G - Q_{AM} + Q_e + \Sigma(m\bar{C}_P)_R\ (T_i - T_R) - \Sigma(m\bar{C}_P)_P (T_o - T_R) - \Delta H_R \tag{5}$$

For a trial value of T_{MOD}', Q_{AM} is calculated by subroutine QSURR. Equation (5) is solved for PHI. Subroutine ESTIM is then used to determine the value of T_{MOD}' for which PHI equals zero. Convergence is satisfied when

$$\left| \frac{PHI}{Q_e + \Sigma(mC_p)_R\ (T_i - T_R)} \right| < \frac{R(75)}{100.} \qquad (6)$$

4.0 Lower Level Subroutines and Functions

QSURR
ESTIM

5.0 References:

1. Brown, D. L. "Investigation of an Electrochemical Device for Carbon Dioxide Absorption and Oxygen Generation". ASD TDR 63-441, May 1963 (Ionics)

2. Brown, D. L. et al.: "Performance of an Electrochemical Device for Simultaneous Carbon Dioxide Removal and Oxygen Generation", Chem. Engr. Progress Symposium Series, No. 63, Vol 62 (1966), p. 50.

H2DP0L

Component Subroutine No. 32 - Hydrogen Depolarized Cell

1.0 Subroutine Description

This subroutine is used to simulate a hydrogen depolarized cell for CO_2 concentration. The cell operates as a fuel cell consuming hydrogen and oxygen to produce water and electricity. Along with this process CO_2 is removed from a cabin air stream passing through the cathode compartment of the cell. The CO_2 is removed by absorption and chemical reaction in a $Cs_2\ CO_3$ electrolyte. The CO_2 is reformed in the anode compartment by reaction of $CO_3^=$ ions with water. CO_2 is swept out along with unreacted hydrogen which flows through the compartment. The hydrogen gas depolarizes the electrode causing a shift in the chemical equilibrium in a direction favorable to reformation of the CO_2.

Figure 1 illustrates the principal electro-chemical reactions occurring in the cell. As can be seen from the figure, purified air flows out of the cathode compartment. A CO_2/H_2 mixture plus water vapor flows out of the anode compartment. By careful regulation of operating conditions, effective CO_2 collection can be accomplished while providing a suitable feed to a Sabatier reactor. Hence, H_2 and CO_2 react to form CH_4 and H_2O. The H_2O can then be electrolyzed to reform oxygen.

This subroutine is a slightly modified version of a subroutine prepared by Hamilton Standard for simulation of the unit prepared for the SSP program. A complete documentation of this routine is given in reference 1.

2.0 SUBROUTINE DATA

2.1 General Notes

1. A flow code of 2 or 3 must be specified for the primary side of this component. The inlet flow to the primary side is assumed to be the air stream which is to be stripped of CO_2.

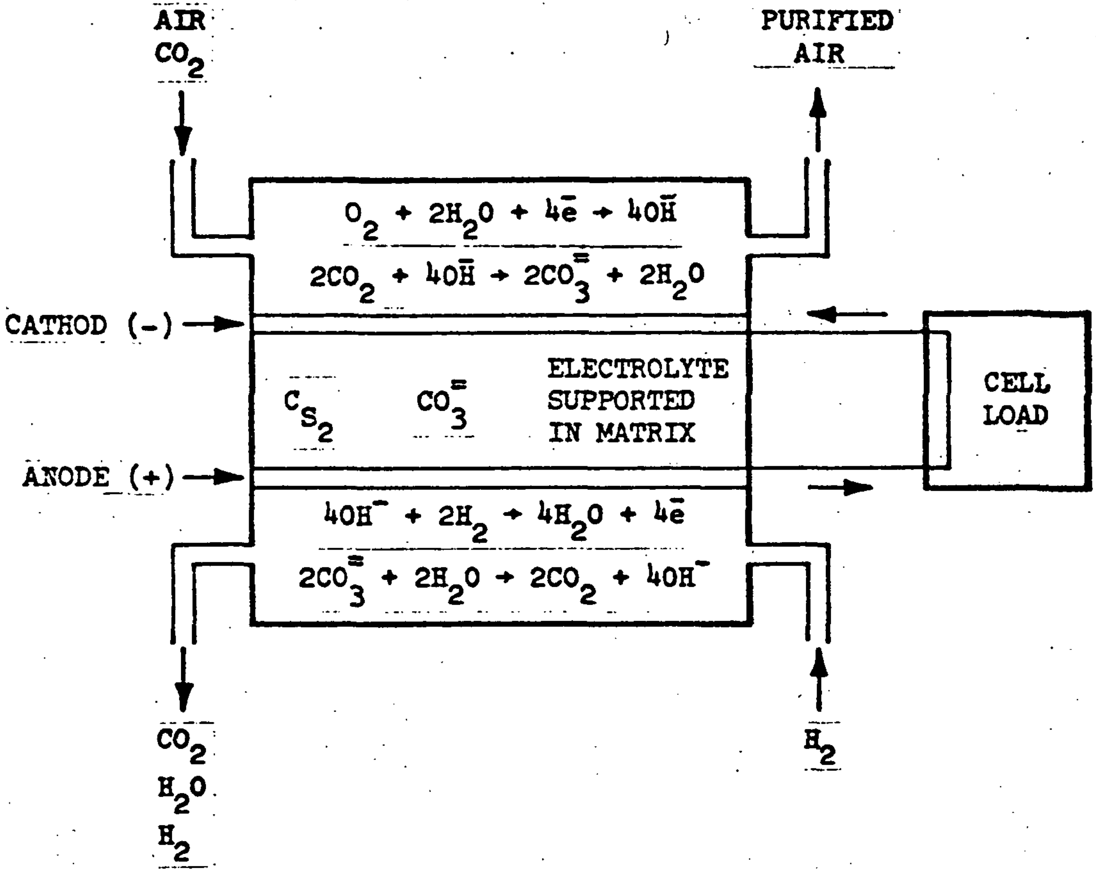


FIGURE 1. HYDROGEN DEPOLARIZED CELL

2. A flow code of 3 must be specified for the secondary side of this component. The inlet flow to the secondary side is assumed to be hydrogen plus some water vapor. Hydrogen enters as special flow no. 1.

3. The subroutine contains logic which will determine the desired condition of the electrolyte in order to meet system constraints on inlet CO_2 partial pressure, process flow rate, total pressure, operating temperatures, and dew point. The electrolyte condition is then defined in terms of the following:

   - Partial pressure H_2O in electrolyte
   - Weight of H_2O in electrolyte
   - Maximum allowable electrolyte specific volume
   - Minimum allowable electrolyte specific volume
   - Maximum allowable electrolyte volume

The computer logic for determining the electrolyte condition will be performed once at the beginning of each new transient case. For CHANGE cases not starting from zero time, the logic will be performed if an integer instruction in K (NK+22) is set greater than zero. After the logic is performed, the instruction will be automatically set to zero.

2.2 Steady-State K Array Data

Reference Location	Description	Data Type
16	Table number for partial pressure water vapor (mmHg) 1st independent variable = electrolyte concentration (wt %) 2nd independent variable = temperature (°F)	

Reference Location	Description	Data Type
17	Table number for electrolyte concentration (wt %) 1st independent variable = temperature (°F) 2nd independent variable = partial pressure water vapor (mm Hg)	
18	Table number of electrolyte specific conductance $(\text{ohm-cm})^{-1}$ 1st independent variable = temperature (°F) 2nd independent variable = electrolyte concentration (wt %)	
19	Table number for electrolyte concentration (wt %) versus electrolyte molarity (g moles/liter)	
20	Table number for electrolyte molarity (g moles/liter) versus electrolyte concentration (wt %)	
21	Table number for electrolyte specific volume (cm^3/gram electrolyte) versus electrolyte concentration (wt %)	
22	Table number for Reynold's factor ( ) versus friction factor ( ).	
23	Integer instruction to determine initial condition of electrolyte on first pass of a transient run 0 no 1 yes	

2.3 Steady State and Transient V Array Data

Reference Location	Description	Data Type
65	Maximum cabin CO_2 partial pressure (mm Hg)	I(R)
66	Cell temperature at time zero (°F)	I(R)

Reference Location	Description	Data Type
67	Lowest air temperature for operation (°F)	I(R)
68	Maximum air pressure for operation (psi)	I(R)
69	Maximum air flow rate for operation (cfm)	I(R)
70	Maximum air water vapor partial pressure for operation	I(R)
71	Cell length (ft)	I(R)
72	Total width of all cells (ft)	I(R)
73	Air channel dimension (in)	I(R)
74	Current collector width (in)	I(R)
75	Electrode spacing (mils)	I(R)
76	Matrix thickness before compression (mils)	I(R)
77	Matrix void volume fraction	I(R)
78	Total mass of cell stack (lb)	I(R)
79	Average Cp of cell stack (Btu/lb-°F)	I(R)
80	Available sponge vol. per ft^2 of matrix area (ml/ft^2)	I(R)
81	Maximum electrolyte specific volume (cm^3/gram)	0
82	Minimum electrolyte specific volume (cm^3/gram)	0
83	Total mass H_2O in electrolyte at time zero (lb)	0
84	Partial pressure of water vapor in electrolyte at time zero (mm Hg)	0
85	Average cell temperature (°F)	0
86	Current efficiency for CO_2 processing (fraction)	0
87	Total current (amps)	0

Reference Location	Description	Data Type
88	Power output from cell (watts)	0
89	Rate of H_2 consumption (lb/hr)	0
90	Rate of O_2 consumption (lb/hr)	0
91	Average electrolyte concentration (wt %)	0
92	Specific volume of electrolyte (cm^3/gram)	0
93	Air side pressure drop across cell (psi)	0
94	H_2 partial pressure in cell (mm Hg)	0
95	CO_2 partial pressure in cell (mm Hg)	0
96	H_2O partial pressure in cell (mm Hg)	0
97	Volume flow rate of gas to Sabatier reactor (cfm)	0
98	Partial pressure of CO_2 in outlet air stream (mm Hg)	0
99	Partial pressure of H_2O in outlet air stream (mm Hg)	0
100	Cell current (amps)	0
101	Cell voltage (volts)	0
102	Heat generated in cell stack (Btu/hr)	0
103	Air side Reynolds number	0
104	Average heat transfer coefficient cell to process gas (Btu/hr ft^2-°F)	0
105	Bed temperature (°F)	0
106	Partial pressure of H_2O in bed (mm Hg)	0
107	Catholyte concentration (wt %)	0
108	Electrolyte conductivity $(\text{ohm cm})^{-1}$	0
109	Dimensionless number used in calculation of electrolyte concentration (dimensionless)	0

Reference Location	Description	Data Type
110	Cell voltage (volts)	0
111	Total heat generated in cell stack (Btu/hr)	0
112	Air flow Reynolds number (dimensionless)	0
113	Average heat transfer coefficient cell to process gas (Btu/hr-ft^2-°F)	0
114	Electrolyte conductivity (ohm cm)$^{-1}$	0
115	Catholyte concentration (wt %)	0
116	Electrolyte concentration (moles/liter)	0
117	Available sponge volume (cm^3 or ml)	0
118	Matrix factor (dimensionless)	0
119	Maximum electrolyte volume (cm^3)	0
120	Minimum electrolyte volume (cm^3)	0
121	Total H_2O in electrolyte at time t (lb)	0
122	Partial pressure H_2O in electrolyte at time t (mm Hg)	0
123	Total CS_2 CO_3 in cell stack (lb)	0
124	Average friction factor (dim.)	0
125	Reciprocal of (area) * (modified heat transfer coefficient) (hr °F/Btu)	0
126	(Area) * (mass transport coefficient) (lb/hr mm Hg)	0
127	Variable used in calculation of electrolyte concentration (dimensionless)	0
128	CO_2 removal rate (lb/hr)	0
129	An indicator for the operating mode of the unit 0. unit is off 1. unit is on	0

3.0 ANALYTICAL MODEL DESCRIPTION

A complete description of the mathematical model used for subroutine is given in reference 1.

4.0 LOWER LEVEL SUBROUTINES AND FUNCTIONS

VALUE
PRØP
FLØSUM
SK

5.0 REFERENCES

1. "Hydrogen Depolarized Cell CO_2 concentrator Computer Program Simulation", William J. Ayotte, September 10, 1971. NASA MSC Document

LIQCON

Component Subroutine No. 52 - Liquid Contactor

1.0 Subroutine Description

This subroutine simulates the liquid contactor of a liquid absorption CO_2 concentrator subsystem. In the contactor, a cabin air stream is mixed with an aqueous carbonate solution to promote absorption of CO_2 from the gas phase into the aqueous liquid phase. Either a potassium or sodium cabronate/bi-carbonate solution may be used for the liquid phase. The absorption of CO_2 is promoted by chemical reaction of the absorbed CO_2 with the carbonate solution to form bi-carbonate. The absorption reaction is favored when the temperature is approximately room temperature. Desorption or reversal of the chemical reaction can be achieved by heating the solution to approximately 180°F.

A suitable zero-g design has not been defined at this time. Counter-current flow is commonly used in industrial gas/liquid absorption processes. However, it is difficult to envision a counter flow contactor for zero-g operation. For this reason, the contactor has been assumed to be designed for co-current or parallel operation.

Reference 1 has suggested ceramic saddle packing for promoting contact of the gas/liquid phases. A detailed transient simulation of this type of component would involve setting up macroscopic mass and energy balances for bed elements in the direction of the flow. In order to predict the mass transfer rate, mass transfer coefficients for both the liquid and gas phases would be required. Since a suitable contactor design is undefined at this time, a detailed analytical model of the nature described above is not warranted. However, by assuming parallel flow and that the bed is long enough for the gas and liquid phases to be in equilibrium, a suitable math model can be prepared. This provided the basis for the subroutine prepared.

Figure 1 shows the inlet and outlet streams for the contactor. Since the contactor is assumed to be operating under zero-g conditions, the outlet stream is assumed to be a mechanical mixture of gas and entrained liquid. An additional device for gas/liquid separation is assumed to be located downstream of the contactor.

2.0 Subroutine Data

2.1 General Notes

1. A flow code of 3 must be specified for the primary side of the component.
2. The source of primary flow to the component must have a flow code of 2 or 3. The source of secondary flow must have a flow code of 4.
3. For the secondary flow, special flow number 2 is assumed to be liquid water. Special flow 3 is carbonate and special flow 4 is bi-carbonate. The total flow is the sum of special flows 2, 3, and 4.
4. For the primary flow leaving the component, special flow number 2 is entrained water, special flow 3 carbonate, and special flow 4 is bi-carbonate. R(07) is set equal to zero. The gas phase is assumed to be saturated with water vapor. R(06) is set equal to this flow. The flows of remaining constituents of the gas phase are inserted in R(10) through (13).
5. The gas flow entering the liquid contactor should have a high relative humidity to prevent evaporative losses in the contactor.

2.2 Instruction Options

NSTR(1): Specifies type of base in liquid
= 0 Potassium carbonate/bi-carbonate
= 1 Sodium carbonate/bi-carbonate

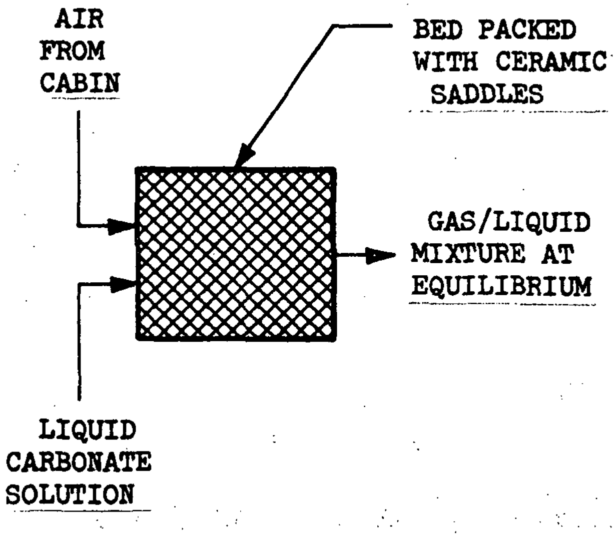


FIGURE 1 LIQUID CONTACTOR FOR CO_2 ABSORPTION

NSTR(2): Specifies an option for determining the liquid flowrate required.

= 0 Do not determine required liquid flowrate

= 1 Determine liquid flowrate required to meet CO_2 removal efficiency specified in R(65)

2.3 Steady State V-Array Data

Reference Location	Description	Data Type
R(65)	The CO_2 removal efficiency of the liquid contactor (fraction)	I(R) if NSTR(2)=0 otherwise, 0
R(66)	CO_2 removal rate from cabin air stream (lb/hr)	
R(77)	Fraction of base that is bicarbonate in liquid entering contactor (weight fraction)	
R(68)	The normality of the base flowing into the contactor $\frac{\text{gram equivalents}}{\text{liter of solution}}$	
R(69)	Equilibrium partial pressure of CO_2 leaving the contactor (mmHg)	0
R(70)	Fraction of base that is bicarbonate in liquid leaving the contactor (weight fraction)	0
R(71)	Mass of water evaporated into the gas phase (lb/hr)	0

3.0 Analytical Model Description

The CO_2 removal rate is predicted for parallel flow of gas and liquid phases in a packed absorption bed. The bed is assumed to be sufficiently long for the gas and liquid phases to be in equilibrium. The equilibrium relationship for the gas and liquid at the exit of the contactor is given in reference 2 as follows:

for potassium carbonate:

$$P_{CO_2,o} = \frac{45\, f_o^{2}\, N^{1.29}}{S(1-f_o)(302-t)} \qquad (1,a)$$

for sodium carbonate:

$$P_{CO_2,o} = \frac{137\, f_o^{\,2}\, N^{1.29}}{S(1-f_o)(365 - t)} \qquad (1,b)$$

where:

$P_{CO_2,o}$ = partial pressure of CO_2 in exit gas leaving contactor (mmHg)

t = temperature of liquid or gas (°F)

f_o = fraction of total base that is bicarbonate in liquid leaving the contactor $\left(\frac{\text{lb of base (i.e., sodium) as bi-carbonate}}{\text{total lb of base (i.e., sodium)}}\right.$

S = solubility of CO_2 in H_2O at one atmosphere (gram moles CO_2/liter H_2O

N = normality of base $\left(\frac{\text{gram equivalents}}{\text{liter}}\right)$

A least squares fit of data from reference 2 was obtained for solubility versus temperature.

$$S = A_1 + A_2t + A_3t^2 + A_4t^3 + A_5t^4 \qquad (2)$$

where:

A_1 = .14202

A_2 = $-.276085\text{x}10^{-2}$

A_3 = $.2461856\text{x}10^{-4}$

A_4 = $-.104096\text{x}10^{-6}$

A_5 = $.1659179\text{x}10^{-9}$

CO_2 reacts with carbonate solution according to the following reaction:

$$K_2CO_3 + CO_2 + H_2O \longrightarrow 2KHCO_3 \qquad (3)$$

This relationship was used to derive a mass balance equation for transfer between the gas and liquid phases. This relationship is presented below:

$$2\,G\left[\frac{P_{CO_2,\,i}}{P_T - P_{CO_2,\,i}} - \frac{P_{CO_2,\,o}}{P_T - P_{CO_2,\,o}}\right] = L'N\,(f_o - f_i) \times \frac{MW}{1000.} \qquad (4)$$

where:

G = total flowrate of gas (lb moles/hr)

L' = total flowrate of solution (lb moles/hr)

f_o, f_i = fraction of total base that is bicarbonate in solution leaving and entering, respectively (weight fraction)

$P_{CO_2,o}$, $P_{CO_2,i}$ = partial pressure of CO_2 leaving and entering, respectively (mmHg)

P_T = total pressure (mmHg)

MW = molecular weight of water

Equations (2) and (4) are combined to form a quadratic equation which is solved by the standard equation for solution of quadratic equations. The solution yields values for the two unknowns, $P_{CO_2,o}$ and f_o.

An overall thermal balance is performed including the net enthalpy addition due to gas and liquid entering and leaving the contactor, and heat absorbed by vaporization of water into the gas phase. The heat of chemical reaction is considered to be negligible.

4.0 Lower Level Subroutines and Functions

PSAT

5.0 References:

1. "Mars Landing and Reconnaissance Mission Environmental Control and Life Support System Study", Hamilton Standard, 1964, p 2-30.
2. Perry, R. H., "Chemical Engineer's Handbook", 4th Edition, p 14-10 McGraw-Hill, New York (1960).

LQFLSH

Component Subroutine No. 56 - Liquid Flash Vaporizer

1.0 Subroutine Description

This subroutine simulates the flash vaporizer component of a liquid absorption CO_2 concentrator subsystem. The component is assumed to be connected to a vacuum pump which maintains a pressure low enough to cause partial vaporization of the aqueous carbonate/bicarbonate solution entering. Along with the vaporization process, bicarbonate decomposes into carbonate and CO_2. Thus, a gas phase mixture of H_2O and CO_2 and a liquid mixture of aqueous carbonate/bicarbonate is created. A suitable device is assumed to be available for achieving separation of the two phases.

The subroutine assumes that the exiting gas and liquid phases are in thermodynamic and chemical equilibrium. The vaporization process is assumed to occur at the inlet temperature. The subroutine calculates the amount of heat that must be supplied to maintain this temperature. Effective CO_2 separation can be achieved with a temperature of approximately 180°F.

Figure 1 shows the inlet and outlet stream for the liquid flash vaporizer. The separation of liquid and gas is assumed to occur within the component.

2.0 Subroutine Data

2.1 General Notes

1. A flow code of 4 must be specified for the primary source of the component.
2. There is no secondary source.
3. The primary outlet flow uses a flow code of 4. Special flow number 2 is assumed to be water. Special flow 3 is carbonate and special flow 4 is bicarbonate. The total flow leaving the liquid vaporizer is the sum of special flows 2, 3, and 4.

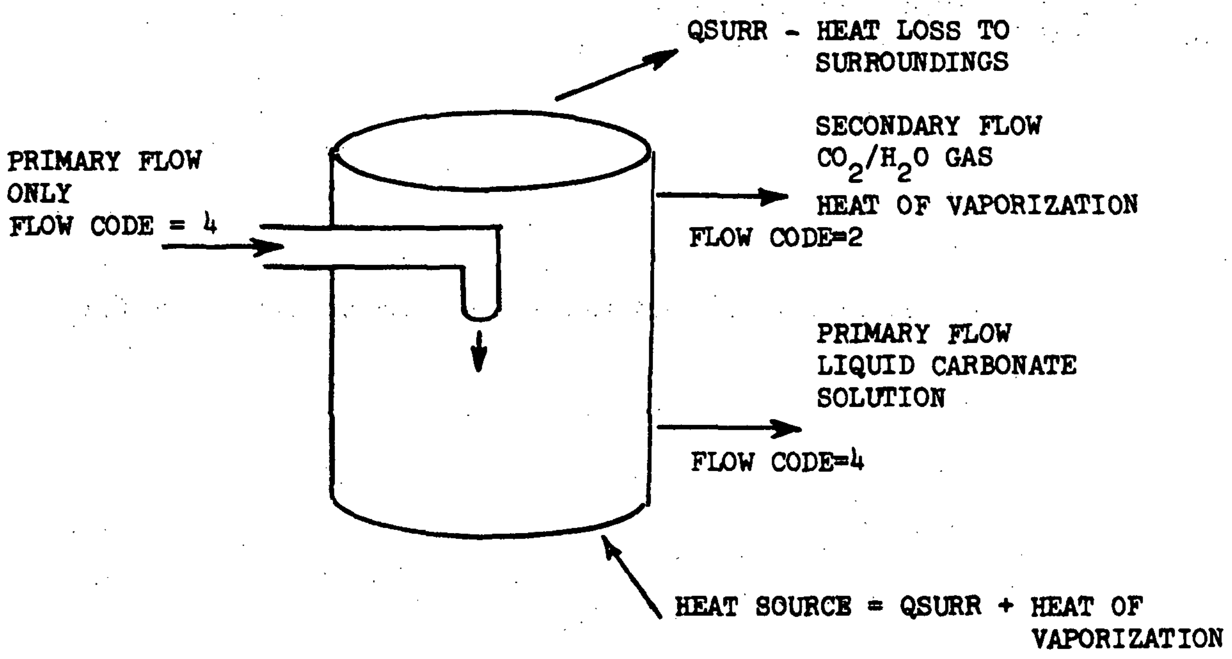


FIGURE 1. LIQUID FLASH VAPORIZER FOR CO_2 DESORPTION

4. The temperatures of the solution and the gas leaving LQFLSH are equal to the temperature of the solution entering.

2.2 Instruction Options

NSTR(1):	Specifies type of base in liquid
= 0	Potassium carbonate/bicarbonate
= 1	Sodium carbonate/bicarbonate

2.3 Heat Loss V-Array Data

Reference Location	Description	Date Type
51	Average flash vaporizer housing temperature (°F)	0
52	Effective summed conductance to ambient (Btu/hr-°F)	0
53	Component total ambient heat loss (Btu/hr)	0
54	Ambient gas temperature (°F)	I(R)
55	Thermal conductance between surface of insulation and ambient gas (Btu/hr-°F)	I(R)
56	Convective heat loss to ambient gas (Btu/hr)	0
57	Ambient radiation wall temperature (°F)	I(R)
58	Thermal radiation A factor from surface of insulation to ambient wall (Ft^2)	I(R)
59	Radiative heat loss to ambient wall (Btu/hr)	0
60	Structure temperature for heat shorts (°F)	I(R)
61	Thermal conductance between flash vaporization module and structure (Btu/hr-°F)	I(R)
62	Conductive heat loss to structure (Btu/hr)	0
63	Insulation surface temperature	0
64	Conductance between module and outer surface of insulation (Btu/Hr-°F). (If R(64) = 0, there is no insulation)	I(R)

2.4 Steady State V-Array Data

Reference Location	Description	Data Type
R(65)	The nominal CO_2 partial pressure in the exit gas flash vaporization module (mmHg)	I(R)
R(66)	Decomposition rate of the bicarbonate yielding CO_2,H_2O and carbonate (lb/hr)	0
R(67)	Fraction of base that is bicarbonate flowing into the liquid flash vaporizer (weight fraction)	0
R(68)	Desired normality of the base leaving the liquid flash vaporizer (g equivalents/liter)	I(R)
R(70)	Fraction of base that is bicarbonate leaving the module (weight fraction)	0
R(71)	Total heat required to maintain temperature at inlet condition (Btu/hr)	0
R(72)	Amount of makeup water required to maintain the normality of carbonate solution specified in R(68) (lb/hr)	0

3.0 Analytical Model Description

When hot, aqueous carbonate/bicarbonate solution is introduced into a low pressure vessel, CO_2 gas will be liberated and a portion of the water vaporized. The gas and liquid phases are assumed to leave the vessel in thermodynamic and chemical equilibrium. The subroutine uses an iterative procedure to determine the total gas and liquid flows and molar concentrations for equilibrium conditions. The method used is outlined as follows:

1. The CO_2 partial pressure in the exit gas is assumed to be controlled to a specified value by means of a vacuum pumping system. The fraction bicarbonate in a solution in equilibrium at this pressure is given by the following relationships:

for potassium carbonate/bicarbonate:

$$P_{CO_2,o} = \frac{45 f_o^{2} N^{1.29}}{S(1-f_o)(302-t)} \qquad (1,a)$$

for sodium carbonate/bicarbonate:

$$P_{CO_2,o} = \frac{135 f_o^{2} N^{1.29}}{S(1-f_o)(365-t)} \qquad (1,b)$$

where:

$P_{CO_2,o}$ = partial pressure of CO_2 in gas phase leaving vaporizer (mmHg)

t = temperature of liquid and gas phases leaving vaporizer (F)

f_o = fraction bicarbonate in liquid stream leaving
$\frac{\text{lb of base (i.e., sodium) as bicarbonate}}{\text{total lb of base (i.e., sodium)}}$

N = normality of base in stream leaving $\frac{\text{g equivalents}}{\text{liter}}$

S = solubility of CO_2 in H_2O at one atmosphere $\frac{\text{g moles } CO^2}{\text{liter } H_2O}$

Data from reference 1 was used to obtain a polynominal relationship for S

$$S = A_1 + A_2 t + A_3 t^2 + A_4 t^3 + A_5 t^4 \qquad (2)$$

where:

$A_1 = .14202$

$A_2 = -.276085 \times 10^{-2}$

$A_3 = .2461856 \times 10^{-4}$

$A_4 = -.104096 \times 10^{-6}$

$A_5 = .1659179 \times 10^{-9}$

2. Assuming the liquid normality remains constant, the fraction bicarbonate in the exit stream can be determined by equations (1,a) or (1,b). Knowing the inlet and outlet fraction bicarbonate and the total amount of base entering, the amount of bicarbonate reacting, and CO_2 generated, can be determined by the reactions chemical mass balance equations

$$2\ HCO_3^- \rightleftarrows CO_3^= + H_2O + CO_2 \qquad (3)$$

The mole fractions of each constituent in the liquid phase can then be calculated.

3. Using Henry's law, the equilibrium partial pressure for water vapor is determined. This is added to the CO_2 partial pressure to obtain the total pressure. The mole fraction of each constituent in the gas phase is then determined by the ideal gas law.

4. Knowing the molar flow rate of CO_2 (from eq. 3) and the mole fraction CO_2 and H_2O in the gas phase, the molar flow rate of H_2O in the exit gas can be determined by Dalton's law.

5. A new estimate for the normality of the exit solution is made and the above procedure is repeated until convergence is obtained within an acceptable tolerance.

After determining the outlet flows for the flash vaporization, the subroutine determines the amount of makeup water required to achieve the desired normality specified in R(68). The amount of process heat that must be supplied to maintain the outlet temperature equal to the inlet temperature is also determined. This heating is assumed to be supplied by a heating coil inside the vaporizer.

4.0 Lower Level Subroutines and Functions

PSAT
QSURR
HG

5.0 References

1. Perry, R. H., "Chemical Engineers' Handbook", 4th Edition, p 14-10, McGraw-Hill, New York (1960).

MEMOD

Component Subroutine No. 55 - Membrane Module Subroutine

1.0 Subroutine Description

This subroutine simulates the transport across membranes (membrane permeation) of selected gasses such as CO_2, N_2, O_2 and H_2O. Membrane permeation is a concentration process accomplished by selective diffusion of a specified gas due to a partial pressure gradient.

The membrane module consists of membranes packaged in multiple layers with intervening backing screens. The supply gas or feed gas is forced laterally through every other screen and the "sweep gas" used for the removal of diffusing constituent is forced through the alternate screens. The critical parameter for determining the diffusion rate of a gas through a membrane is its permeability which is defined as follows:

$$[\text{Perm}] = \frac{(\text{Volumetric Flow(STP)})\ (\text{Membrane thickness})}{(\text{Membrane area})\ (\text{Pressure Differential})}$$

Concurrently with the mass transfer of gasses that occurs, thermal energy is also transferred through the membrane and through the module housing. Since the thickness of the membrane is small, the thermal conductance through the membrane is very large in comparison to the heat transfer coefficient of both sides of the membrane. Thus, only the convective heat transfer coefficients are considered in evaluating the heat flow through the membrane. This subroutine models the heat flow to the housing and from housing to the surroundings by working with only one housing temperature which is assumed to be the average temperature.

The subroutine is generalized in that there are no restrictions on type of feed or sweep gases. In addition to having the capability of simulating diffusion of species mentioned above, the program also can simulate the diffusion of one special flow species. Thus such processes such as hydrogen separation through a semi-permeable membrane may be simulated.

While the mathematical model described in Section 3.0 is described in terms of rectangularly shaped cells, any regular shaped cell can be handled. For instance a cell consisting of concentric cylinder with feed gas flowing in the inner cylinder and sweep gas in the annular can be simulated.

Figure 1 illustrates a gas separation module with multiple number of rectangular shaped cells. This configuration is simulated by specifying the characteristic dimensions of a membrane cell and the number of membrane cells. The characteristic dimensions required are the cell frontal areas and the length, the area of membrane separating the cell pair, and the thickness of the membrane.

A cell with a vacuum on one side, rather than sweep gas, may also be simulated. Here a dummy flow must be supplied to the side with the vacuum which will always be the secondary side. Actually, this is the flow out of the cell as determined by a vacuum pump. A special option (NSTR(1)=1) must be flagged to instruct the program that no flow is entering the secondary side of the cell.

2.0 Subroutine Data

2.1 General Notes

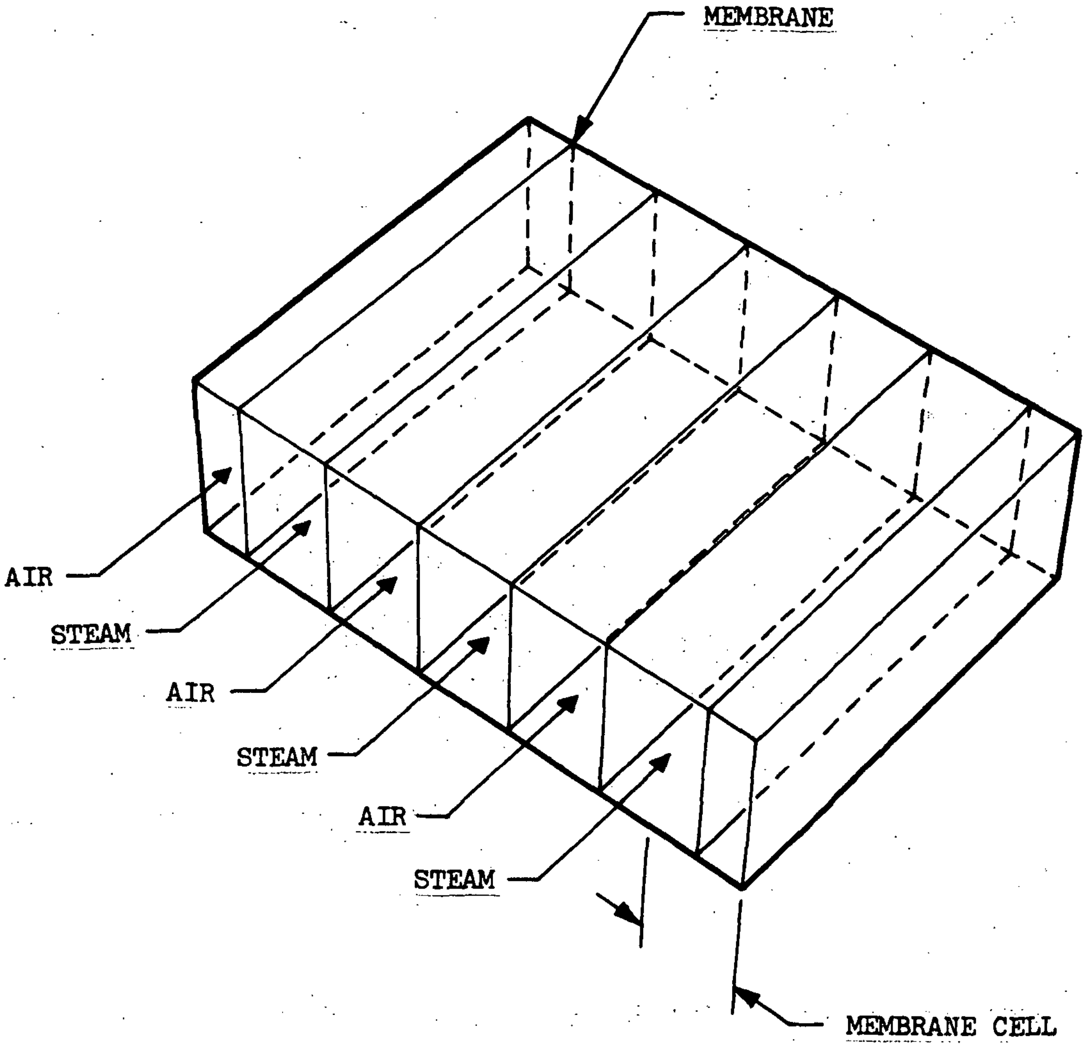
1. Only flow codes 1,2, or 3 are allowed by the subroutine. The program deals with diffusion of gases through a membrane.
2. A certain level of non-condensable flow must always be specified in both sides of the module.
3. This subroutine can compute diffusion rate of 6 gas species simultaneously, provided that the permeability factors of each component gases are input. Excluding the permeability factors for any component gases is equivalent to setting the value to zero.

2.2 Instruction Options

NSTR(1):	Secondary side is connected to a vacuum pump
= 0	Secondary side is not connected to a vacuum pump
= 1	Secondary side is connected to a vacuum. The diffused gas is removed by using a vacuum pump. A dummy secondary flow must be provided which is actually the flow out of the cell. This flow should be calculated using the vacuum pump subroutine (VACPMP)

2.3 Steady State K-Array Data

Reference Location	Description	Data Type
16	Total number of membrane cells in the module, NMEM. (If the number is not input the value is assumed to be one). Figure 1 illustrates the definition of membrane cells.	I(R)



MEMBRANE CELL EXAMPLE:
6 MEMBRANES
3 STEAM CELLS
3 AIR CELLS, 2 HALFS + 2 FULL
MEMBRANE CELLS = MEMBRANES = 6

FIGURE 1 ILLUSTRATION OF A GAS SEPARATION MODEL USING MEMBRANES

2.4 Heat Loss V-array Data

Reference Location	Description	Data Type
51	Avg. Temperature of the housing wall (°F)	0
52	Effective thermal conductance from the module wall	0
53	Total heat loss to surroundings (Btu/hr) R(53)= R(56)+ R(59)+R(62)	0
54	Ambient gas temprature (°F)	I(R)
55	Thermal conductance (UA) between surface of insulation and ambient gas (Btu/hr-°F)	I(R)
56	Convective heat loss to ambient gas (Btu/hr)	0
57	Ambient wall temperature (°F)	I(R)
58	FA between ambient wall and surface of insulation(Ft^2)	I(R)
59	Radiative heat loss to ambient wall (Btu/hr)	0
60	Structure temperature (°F)	I(R)
61	Conductance (KA/X) between module and structure (Btu/hr-°F)	I(R)
62	Conductive heat loss to structure (Btu/hr)	0
63	Insulation surface temperature (°F)	0
64	Conductance (KA/X) between the module housing and outer surface of insulation Btu/hr-°F) (If R(64)=0, there is no insulation)	I(R)

2.5 Steady State V-Array Data

Reference Location	Description	Data Type
65	Membrane area for a cell. Total area for the module is obtained by multiplying number of cells with the membrane area. (Ft^2)	I(R)
66	Membrane thickness. (inches)	I(R)
67	Oxygen permeability through the membrane $\frac{(Ft^3/hr\ (STP))\ (inches)}{(Ft^2)\ (mmHg)}$	I(R),if the value is not input then diffusion
68	Diluent (normally nitrogen) permeability through the membrane $\frac{(Ft^3/hr\ (STP))\ (inches)}{(Ft^2)\ (mmHg)}$	

Reference Location	Description	Data Type
69	Carbon dioxide permeability through the membrane $\frac{(Ft^3/hr\ (STP))\ (inches)}{(Ft^2)\ (mmHg)}$	of this species is not considered
70	Trace contaminant permeability through the membrane $\frac{(Ft^3/hr\ (STP))\ (inches)}{(Ft^2)\ (mmHg)}$	
71	Special flow #1 permeability through the membrane $\frac{(Ft^3/hr\ (STP))\ (inches)}{(Ft^2)\ (mmHg)}$	
72	Water vapor permeability through the membrane $\frac{(Ft^3/hr\ (STP))\ (inches)}{(Ft^2)\ (mmHg)}$	
73	Oxygen concentration of effluent gas stream, primary side. (mole fraction)	0
74	Diluent (N_2) concentration of effluent gas stream, primary side. (mole fraction)	0
75	Carbon dioxide concentration of effluent gas stream, primary side (mole fraction)	0
76	Trace contaminant concentration of effluent gas stream, primary side. (mole fraction)	0
77	Special flow #1 concentration of effluent gas stream, primary side. (mole fraction)	0
78	Water vapor concentration of effluent gas stream, primary side. (mole fraction)	0
79	Oxygen concentration of effluent gas stream, secondary side. (mole fraction)	0
80	Diluent concentration of effluent gas stream, secondary side. (mole fraction)	0
81	Carbon dioxide concentration of effluent gas stream, secondary side. (mole fraction)	0
82	Trace contaminant concentration of effluent gas stream, secondary side. (mole fraction)	0
83	Special flow #1 concentration of effluent gas stream, secondary side. (mole fraction)	0
84	Water vapor concentration of effluent gas stream, secondary side. (mole fraction)	0
85	Oxygen permeation rate through the membrane (lb/hr)	0
86	Diluent permeation rate through the membrane (lb/hr)	0

Reference Location	Description	Data Type
87	CO_2 permeation rate through the membrane (lb/hr)	0
88	Trace contaminant permeation rate through the membrane. (lb/hr)	0
89	Special flow #1 permeation rate through the membrane (lb/hr)	0
90	Water vapor permeation rate through the membrane (lb/hr)	0
91	Thermal conductance (total) between cell gas and module wall, primary side,(Btu/ hr-°F.)	I(R)
92	Thermal conductance (total) between cell gas and module wall, secondary side, (Btu/hr-°F)	I(R)
93	Effective thermal conductance through a membrane (summed) (Btu/hr-°F)	I(R)
94	Effective specific heat of effluent gas, primary side (Btu/lb-°F)	0
95	Effective specific heat of effluent gas, secondary side (Btu/lb-°F)	0
96-100	Locations not used	

2.6 Transient V-Array Data

All of the transient V-array data that is of I(R) type must be input for transient solution; otherwise steady state solution will be used.

Reference Location	Description	Data Type
101	Volume of module (total), primary side,(Ft^3-)	0
102	Volume of module (total), secondary side,(Ft^3)	0
103	Module Length,(Ft.)	I(R)
104	Frontal Area (Free flow area) of a cell primary side (Ft^2)	I(R)
105	Frontal Area (Free flow area) of a cell, secondary side (Ft^2)	I(R)

Reference Location	Description	Data Type
106	Thermal capacitance of module shell (Btu/°F)	I(R)
107	Multiplying factor used in computing stability line increment in forward difference solution of temperatures and concentrations ($0 < \Delta\theta < 1.0$)	I(R)
108	Minimum allowable computing interval (Seconds)	I(R)

3.0 Analytical Model Description

The analytical model description presented in the following describes a membrane cell with heat and mass flowing through/to cell sides A and B.

3.1 Mass Balance

The equation of continuity for gas flowing through a system for constant density, R_A and diffusivity D_{AB} is given as follows:

$$\overbrace{\frac{\partial C_A}{\partial t} + \nu_x \frac{\partial C_A}{\partial x} + \nu_y \frac{\partial C_y}{\partial y} + \nu_z \frac{\partial C_z}{\partial z}}^{\text{Bulk Flow Term}} = \underbrace{D_{AB}\left(\frac{\partial^2 C_A}{\partial x^2} + \frac{\partial^2 C_A}{\partial y^2} + \frac{\partial^2 C_A}{\partial z^2}\right)}_{\text{Diffusion term}} + R_A \qquad (1)$$

where:

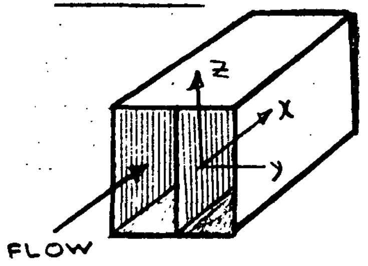
C_A = Concentration $(\frac{lb}{ft^3})$

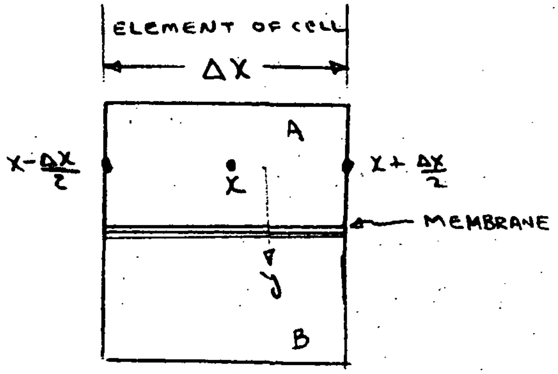
V_i = Velocity $(\frac{Ft}{Sec})$

x,y,z = Length dimensions (ft)

D_{AB} = Diffusivity (ft^2/hr)

Cell Pair





TOP VIEW

3.1 (Cont)

Assumptions:

1. No chemical reaction, i.e. $R_A = 0$
2. Bulk flow in x direction only, Vy and Vz = 0.
3. Diffusion in y direction only, the diffusion in x direction is negligible, as compared to bulk flow to merit consideration.

Taking into account the forementioned assumptions, equation 1 reduces to

$$\frac{\partial C_A}{\partial t} = -v_x \frac{\partial C_A}{\partial x} + \mathcal{D}_{AB} \frac{\partial^2 C_A}{\partial y^2} \qquad (2)$$

The partial differential in the above equations may be approximated as follows:

$$\left.\frac{\partial C_A}{\partial t}\right|_{x+\Delta x/2} = \left.\frac{C_{A_{t+\Delta t}} - C_{A_t}}{\Delta t}\right|_{x+\Delta x/2} \qquad (3)$$

The bulk transfer term:

$$v_x \left.\frac{\partial C_A}{\partial x}\right|_x = v_x \left.\frac{C_{A,x+\Delta x/2} - C_{A,x-\Delta x/2}}{\Delta X}\right|_x \qquad (4)$$

and the diffusion term:

$$\begin{aligned} \mathcal{D}_{AB} \left.\frac{\partial^2 C_A}{\partial y^2}\right|_y &= \mathcal{D}_{AB} \left\{ \left.\frac{\partial C_A}{\partial y}\right|_{y+\Delta y/2} - \left.\frac{\partial C_A}{\partial y}\right|_{y-\Delta y/2} \right\} \\ &= \frac{\mathcal{D}_{AB}}{\Delta y} \left\{ \frac{(C_{A\,y+\Delta y/2} - C_{A\,y}) - (C_{A\,y} - C_{A\,y-\Delta y/2})}{\Delta y} \right\} \end{aligned} \qquad (5)$$

letting Ca = C, and rewriting equation 2 using 3, 4, and 5

$$\begin{aligned} \frac{C_{t+\Delta t} - C_t}{\Delta t} &= \frac{v_x (C_{x-\Delta x/2} - C_{x+\Delta x/2})}{\Delta X} \\ &\quad + \frac{\mathcal{D}_{AB}}{\Delta y} \left\{ (C_{y+\Delta y/2} - C_y) + (C_{y-\Delta y/2} - C_y) \right\} \end{aligned} \qquad (6)$$

for a membrane module cell equation 6 may be written for each diffusing constituent:

$$\frac{C_o' - C_o}{\Delta t} V = Q\,(C_i - C_o) + \frac{D'_{AB}}{\Delta y} A(C^* - Co) \qquad (7)$$

where:

Q = Total volumetric flowrate (Ft^3/hr)

C_i = Concentration of constituent entering cell (lb/Ft^3)

Co = Concentration of constituent leaving the cell, also the concentration in the cell (lb/Ft^3)

C^* = Concentration of constituent on the other side of the membrane (lb/Ft^3)

D_{AB} = Effective diffusivity of gas

A = Membrane area (Ft^2)

Since the resistance to diffusion in the gas phase is negligible compared to the diffusional resistance of the membrane, the effective diffusivity defined above is equal to the permeability of the membrane.

For transient analysis,equation (7) is applied to all diffusing species on both sides of the membrane. For steady state conditions, the equation reduces to the following:

for side A $$0 = Q_A(C_{i,A} - Co_{,A}) + \frac{D'_{AB}A}{\Delta y}(Co_{,B} - Co_{,A}) \qquad (8)$$

for side B $$0 = Q_B(C_{i,B} - Co_{,B}) + \frac{D'_{AB}A}{\Delta y}(Co_{,A} - Co_{,B}) \qquad (9)$$

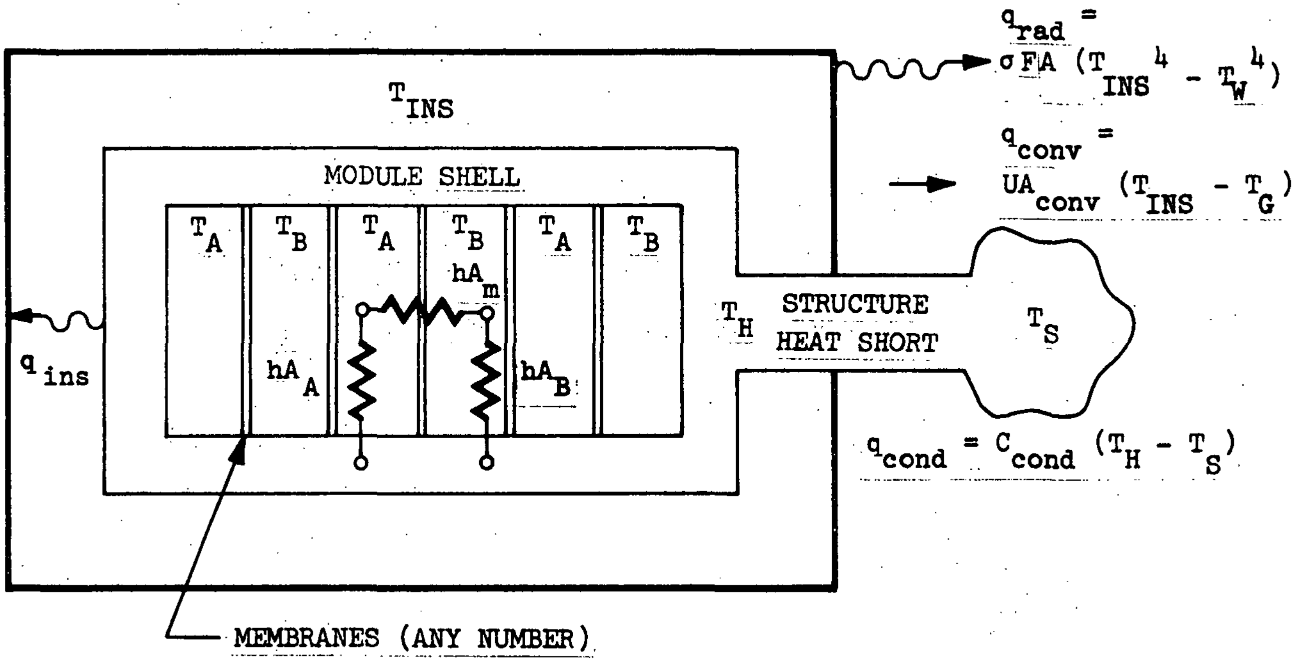
Equations 8 and 9 are solved simultaneously for $Co_{,A}$ and $Co_{,B}$

The transient solution requires a test which determines if the minimum computed time interval is smaller than the minimum allowed computing interval. The stability time increment is computed for each gas species diffusing through the membrane. A steady state solution is used for those with minimum computing interval less than the specified minimum allowable time increment.

3.2 Thermal Balance

Heat transferred through the membrane and heat losses to the surroundings, radiation, convection and conduction are modeled. A schematic drawing of a membrane module is shown in Figure 2. Figure 3 shows the transient lumped parameter nodal network.

PARAMETERS THAT ARE "A" SUBSCRIPTED PERTAIN TO PRIMARY SIDE OF THE MODULE WHILE "B" SUBSCRIPTED PARAMETERS REFER TO THE SECONDARY SIDE OF THE MODULE.



$$q_{INS} = UA_{INS} (T_H - T_{INS}) = q_{conv} + q_{rad}$$

$$q_{surr} = q_{cond} + q_{conv} + q_{rad}$$

$$q_{surr} = hA_A (T_H - T_A) + hA_B (T_H - T_B)$$

$$q_{AB} = hA_m (T_B - T_A)$$

FIGURE 2 THERMAL MODEL FOR MEMBRANE MODULE

R(53) = Total heat loss to surroundings = R(56) + R(59) + R(62)

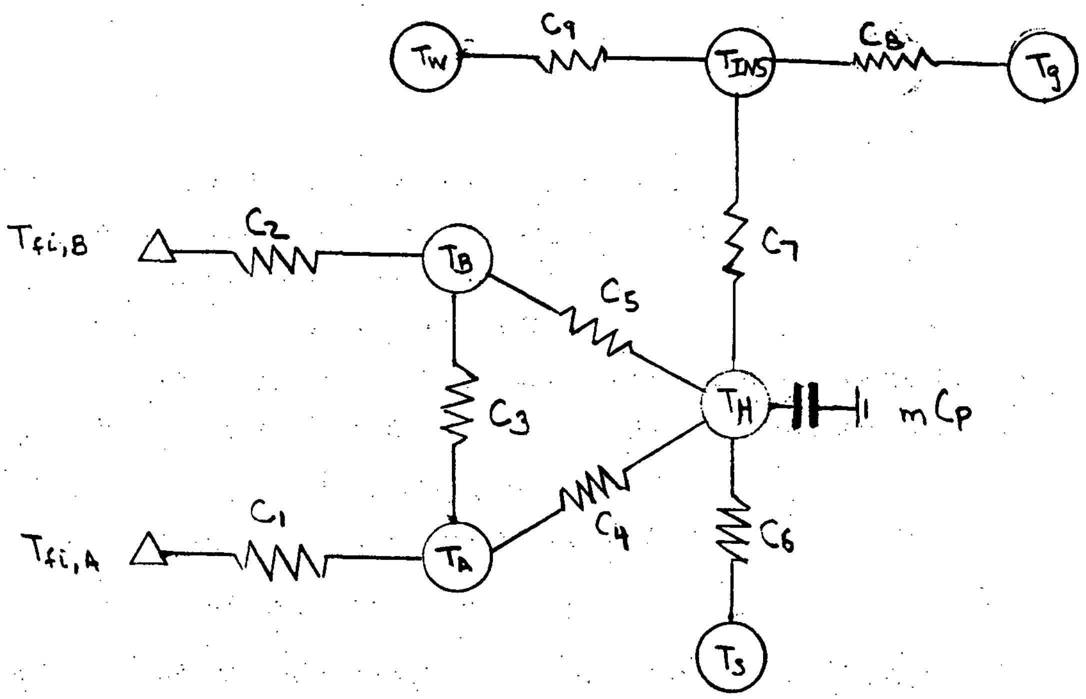
R(59) = Radiative heat loss to ambient wall

$$= FA\ (T_{INS}^{4} - T_{W}^{4})\ , \quad = FA = R(58)$$

R(56) = Convective heat loss to ambient gas

$$= C_8(T_{INS} - T_S) = UA_{conv}\ (T_{INS} - T_g) = R(55)\ (T_{INS} - T_g)$$

R(62) = Conductive heat loss to structure $= C_6(T_H - T_S) = \frac{KA}{X}(T_H-T_S) = R(61)(T_H-T_S)$



T_H = Module Housing Temperature, R(51)

T_{INS} = Temperature of the insulation, R(63)

T_W = Ambient wall temperature, R(57)

T_S = Structure temperature, R(60)

T_A = Fluid temperature in module, also effluent, primary, R(1)

T_B = Fluid temperature in module, also effluent, secondary, R(20)

$T_{fi,A}$ - Primary inlet temperature, A(1)

$T_{fi,B}$ Secondary inlet temperature, B(1)

T_g = Ambient gas temperature, R(54)

mCp = Thermal capacitance of the module housing R(106)

FIGURE 3 LUMPED PARAMETER NODAL NETWORK

The thermal model, as shown in Figure 3, does not take into account the mass transfer through the membrane and does not analyze the rate of energy change of individual gas species. In addition, only the capacitance of the module shell is considered for predicting thermal balance during transient solution.

From Figure 3 we can obtain the following relationships

$$C_1\ (T_{fi,A} - T_A) - C_3\ (T_A - T_B) - C_4\ (T_A - T_H) = 0 \tag{10}$$

and

$$C_2\ (T_{fi,B} - T_B) - C_3(T_B - T_A) - C_5(T_B - T_H) = 0 \tag{11}$$

where:

C_1 = $(w\ C_p)_A$, flow conductance fluid, secondary side, (Btu/hr-°F)

C_2 = $(w\ C_p)_B$, flow conductance fluid, secondary side,(Btu/hr-°F)

C_3 = R(110), thermal conductance through the membrane, (Btu/hr-°F)

C_4 = R(108), conductance between internal fluid and module wall, primary side, (Btu/hr-°F)

C_5 = R(109), conductance between internal fluid and module wall, secondary side,(Btu/hr-F.)

Equations (10) and (11) can be solved simultaneously once the wall temperature T_H is established. An iteration procedure utilizing subroutine QSURR is used to solve the above equations. First the heat loss from the inside of the module to the surface is calculated using equations (10) and (11) for an estimated value of T_H. Using the same estimated value for T_H, the heat loss from the surface to surroundings is determined using subroutine QSURR. Subroutine ESTIM then is used to estimate a better value for T_H. Iterations are continued until convergence is reached.

For transit calculations, the iteration procedure is not required. Here the wall temperature is calculated using the following:

$$\frac{T_H' - T_H}{\Delta t} mC_P = C_4 (T_A - T_H) + C_5(T_B - T_H) - q_{surr} \qquad (12)$$

where:

$m\ C_P$ = thermal capacitance of the tank shell (Btu/°F)

q_{surr} = heat loss to surroundings, computed by QSURR(Btu/hr)

$T_{H'}$, T_H = housing temperature at time $t + \Delta t$ and t respectively (°F)

Δt = compute time interval (hr)

Subroutine MEMOD also accounts for possible condensation of water vapor that may occur in either cell sides, A or B, by computing the effective specific heat. The scheme used by this subroutine is similar to the scheme used by subroutine EFFCP. Details of the procedure are outlined in the EFFCP writeup.

4.0 Lower Level Subroutines and Functions Required

HF (T)

HG (T)

ESTIM (X,Y1,Y11,Y2,Y22,A, NSTR(1))

QSURR
PSAT(T)
TSAT(T)

5.0 References

1. Subroutine EFFCP of Program G189 Manual

MLCARB

Component Subroutine No. 54 - Molten Carbonate Cell

1.0 Subroutine Description

This subroutine is used to simulate the thermodynamic, chemical, and electrochemical processes in a molten carbonate cell. The molten carbonate cell is used for the absorption of CO_2 from cabin air and subsequent conversion to O_2 and C. The device thus is a direct oxygen regeneration subsystem which does not require another subsystem for CO_2 concentration (removal). The chemical and electrochemical reactions occur in a liquified entectic mixture (melt) of LiCl and Li_2O. The process must be operated at a relatively high temperature (550°C) to prevent solidification of the melt.

The mass transfer in the molten state is treated from a quasi-steady state viewpoint. That is, transient diffusional effects are not considered. The cell is treated as a single lumped mass as far as the transient thermal balance is concerned. Heat transfer to the ambient and the enthalpy change for the reaction are included in the temperature balance. Temperature control is achieved primarily by insulation of the housing. The subroutine also allows a miscellaneous heat source to simulate electrical heaters for use in temperature control.

The subroutine makes no assumptions regarding the design concept for the cell. Thus, no assumptions are made concerning the means used for gas/liquid separation.

Many system design parameters for this concept have not been fully defined at this juncture. The composition of the melt, operating temperature, electrode materials and a few of the items which may change before a viable system is evolved. The question of the advisibility of a "dry" or "wet" melt is also unresolved. That is, should the inlet gas be predried to eliminate side reactions involving water vapor? Alternatively, what humidity level should the inlet gas be controlled to for optimum operation. For the subroutine prepared here, the inlet gas is assumed to be dried to a level when water vapor reactions are negligible. Certain additional assumptions were made.

1. The melt is an eutectic mixture of LiCl and Li_2O. Melting point for the mixture is 509°C. Composition is 70% LiCl and 30% Li_2O.
2. Side reactions involving formation of H_2 and CH_4 are ignored.
3. The cathode region is assumed to be shielded to prevent mixing of CO_2 and carbon deposited on the electrode. This will prevent formation of CO which would contaminate the purified air leaving the cell.
4. The anode current density is assumed to be low enough for adequate ionic diffusion. Thus adverse side reactions are prevented which would allow CO_2 contamination of the oxygen generated at the anode.
5. The process is assumed to have 100% current or Faradaic efficiency. Inefficiency due to cell overvoltage and Joule heating are taken into account. The difference between the applied voltage and the theoretical cell voltage times the current results in heat being dissipated in the module. All this heat is assumed to be dissipated in the melt.

2.0 Subroutine Data

2.1 General Notes

1. A primary source flow must be specified to provide an inlet gas flow. The primary side flow code must be 2 or 3. The flow constituents in the source of flow must be compatible with those for the component.
2. The module is assumed to be composed of a number of cells connected in parallel. The number of cells is specified in K(NK+16).
3. A flow code of 2 or 3 must be specified for the secondary side of this component. The secondary flow out of this component will be composed of the oxygen gas generated in the cell.

2.2 Instruction Options

NSTR(1): Specifies method for determining cell voltage

= 0 Cell voltage is calculated from theoretical cell voltage and power efficiency specified in R(69)

= 1 Cell voltage is determined by interpolating a table of values of cell voltage versus current density (amps/ft^2) and cell temperature (°F)

NSTR(2): Specifies method for determining cell current

= 0 Cell current is a constant value input in R(67)

= 1 Cell current required to remove all CO_2 in inlet gas stream is calculated by subroutine

2.3 Heat Loss V-Array Data

Reference Location	Description	Data Type
51	Temperature of module shell (°F)	0
52	Effective thermal conductance from module shell to surroundings (Btu/hr °F)	0
53	Total heat loss to surroundings (Btu/hr) R(53) = R(56) + R(59) + R(62)	0
54	Ambient gas temperature (°F)	I(R)
55	Thermal conductance between surface of insulation and ambient gas (Btu/hr-°F)	I(R)
56	Convective heat loss to ambient gas (Btu/hr)	0
57	Ambient wall temperature (°F)	I(R)
58	Thermal radiation FA from surface of insulation to ambient wall (ft^2)	I(R)
59	Radiative heat loss to ambient wall (Btu/hr)	0
60	Structure temperature (°F)	I(R)
61	Conductance (kA/ΔX) between module shell and structure (Btu/hr)	I(R)

Reference Location	Description	Data Type
62	Conductance heat loss to the structure (Btu/hr)	0
63	Insulation surface temperature (°F)	0
64	Conductance (KA/ΔX) between module shell and outer surface of insulation (Btu/hr-°F)	I(0)

2.4 Steady State K-Array Data

Reference Location	Description	Data Type
16	No. of parallel cells per module	I(R)
17	Table number of cell voltage versus current density (amps/ft^2) and temperature (°F)	I(0)

2.5 Steady State V-Array Data

Reference Location	Description	Data Type
65	Heat dissipated by electrical heater (Btu/hr)	I(0)
66	Heat dissipated in module due to cell inefficiency (Btu/hr)	0
67	Cell current (amps)	I(R) if NSTR(2)=0
68	Cell voltage (volts)	0
69	Power efficiency, η (decimal fraction) $E_{cell} = \frac{E_{theor}}{\eta}$	I(R) if NSTR(1)=1
70	Electrode area (ft^2) per cell	I(R) if NSTR(1)=1
71	Current density (amps/ft^2)	0
72	Convergence tolerance for calculating cell temperature (percent)	I(R)
73	Total CO_2 conversion rate (lb/hr)	0
74	Previous trial value for PHI (Btu/hr)*	0

---

*These quantities are used in the trial and error method used for determining cell temperature. The technique used is described in Section 3.0.

Reference Location	Description	Data Type
75	Previous trial value to T_{cell} (°F)*	0
76	Rate of formation of carbon (lb/hr)	0

2.6 Transient V-Array Data

Reference Location	Description	Data Type
R(77)	Total module thermal capacitance for shell and melt (Btu/°F) (If zero, a steady state solution is used.)	I(0)
R(78)	Cell initial temperature (°F) at time t	I(R)

3.0 Analytical Model Description

The basic chemical and electrochemical reactions occurring at the electrodes of a molten carbonate cell are given below:

at the cathode:

$$4Li^{+} + 4e \longrightarrow 4Li \tag{1}$$

and

$$4Li + CO_2 \longrightarrow 2O^{=} + 4Li^{+} + C \tag{2}$$

or, a net reaction of

$$CO_2 + 4e \longrightarrow 2O^{=} + C \tag{3}$$

at the anode:

$$2O^{=} \longrightarrow O_2 + 4e \tag{4}$$

The net reaction for the complete cell is

$$CO_2 \longrightarrow C + O_2 \tag{5}$$

Using Faraday's law and assuming 100% Faradaic (current) efficiency, the CO_2 decomposition rate is

$$W_{CO_2} = I/1100 \qquad \text{lb } CO_2/\text{hr} \tag{6}$$

---

*These quantities are used in the trial and error method used for determining cell temperature. The technique used is described in Section 3.0.

The cell voltage (neglecting side reactions) is

$$E = 1.025 - \frac{RT}{4F} \ln \frac{P_{CO_2,c}{}^{3}}{\left(P_{O_2,a}\right)\left(P_{CO_2}{}^{2}{}_{,a}\right)} \qquad (7)$$

where

$F = 96,500$ coulombs

$R = 8.312$ international joules/°K-g mole

$T =$ Cell temperature, °F

$P_{CO_2,c} =$ partial pressure of CO_2 at cathode (mmHg)

$P_{CO_2,a} =$ partial pressure of CO_2 at anode (mmHg)

$P_{O_2,a} =$ partial pressure of O_2 at anode (mmHg)

at 550°C and assuming inlet gas partial pressure of 152 and 3.8 mmHg, respectively, for O_2 and CO_2, the cell voltage can be shown (reference 1) to equal

$$E = 1.465 \text{ volts} \qquad (8)$$

The actual cell voltage required has been found to be in the range of 1.6 to 2.0 volts. The subroutine has an option for entering tabular data for cell voltage as a function of current density and cell temperature. Alternatively, the cell voltage can be calculated from the cell efficiency.

$$E_{cell} = {}^{1.025}/\eta \qquad (9)$$

For heat transfer purposes, the module shell and melt are treated as a single lumped mass. Provisions are made for heat losses to the surroundings by conduction to a structure node, and convection and radiation to the ambient. A miscellaneous heat source simulating the input of an electrical heater may be specified. The amount of module insulation is specified by the program user. A schematic for the module thermal model is shown in Figure 1.

The net enthalpy added by the influx and efflux of reactants and products, respectively, and the heat absorbed by chemical reaction also is included in the cell heat balance. Since the enthalpy change is independent of the thermodynamic path chosen, the net enthalpy added to the melt is as follows:

$$\Delta H_T = \left(\overline{NC_P}\right)_R \left(T_{in} - T_o\right) - \left(NC_P\right)_P \left(T_{out} - T_o\right) - \Delta H_{T_o} \left(DCO_2\right) \qquad (10)$$

where:

$\left(\overline{NC_P}\right)_R$ = average hourly heat capacity of reactants (Btu/°F-hr)

$\left(\overline{NC_P}\right)_P$ = average hourly heat capacity of products (Btu/°F-hr)

ΔH_{T_o} = heat of reaction (heat absorbed) at 77°F

= 94,052 x 1.8 (Btu/lb mole CO_2)

DCO_2 = CO_2 reacted (lb mole/hr)

T_o = base temperature for reaction = 77°F

T_{in} = inlet temperature of reactants (°F)

T_{out} = outlet temperature of products (°F)

Rather than using the average specific heats as indicated above, the subroutine uses the integrated enthalpy change for each reactant or product constituent.

$$\Delta H_i = N_i \int_{T_o}^{T} \left(aT^{-2} + bT^{-1} + cT^{o} + dT^{1} + eT^{2} \right) dT \qquad (11)$$

where:

N_i = flow rate of constituent (lb moles/hr)

ΔH_i = enthalpy change for constituent i between temperature T and T_o (Btu/hr)

a,b,c,d = experimentally determined coefficients for heat capacity as a function of temperature. The value of the constants for the major gas constituents in the cell are given in Table I.

The heat balance for the module temperature is given below:

$$\frac{T_{cell}' - T_{cell}}{\Delta \tau} G = -QL\not{O}SS + P + QE + \Delta H_T \qquad (12)$$

where:

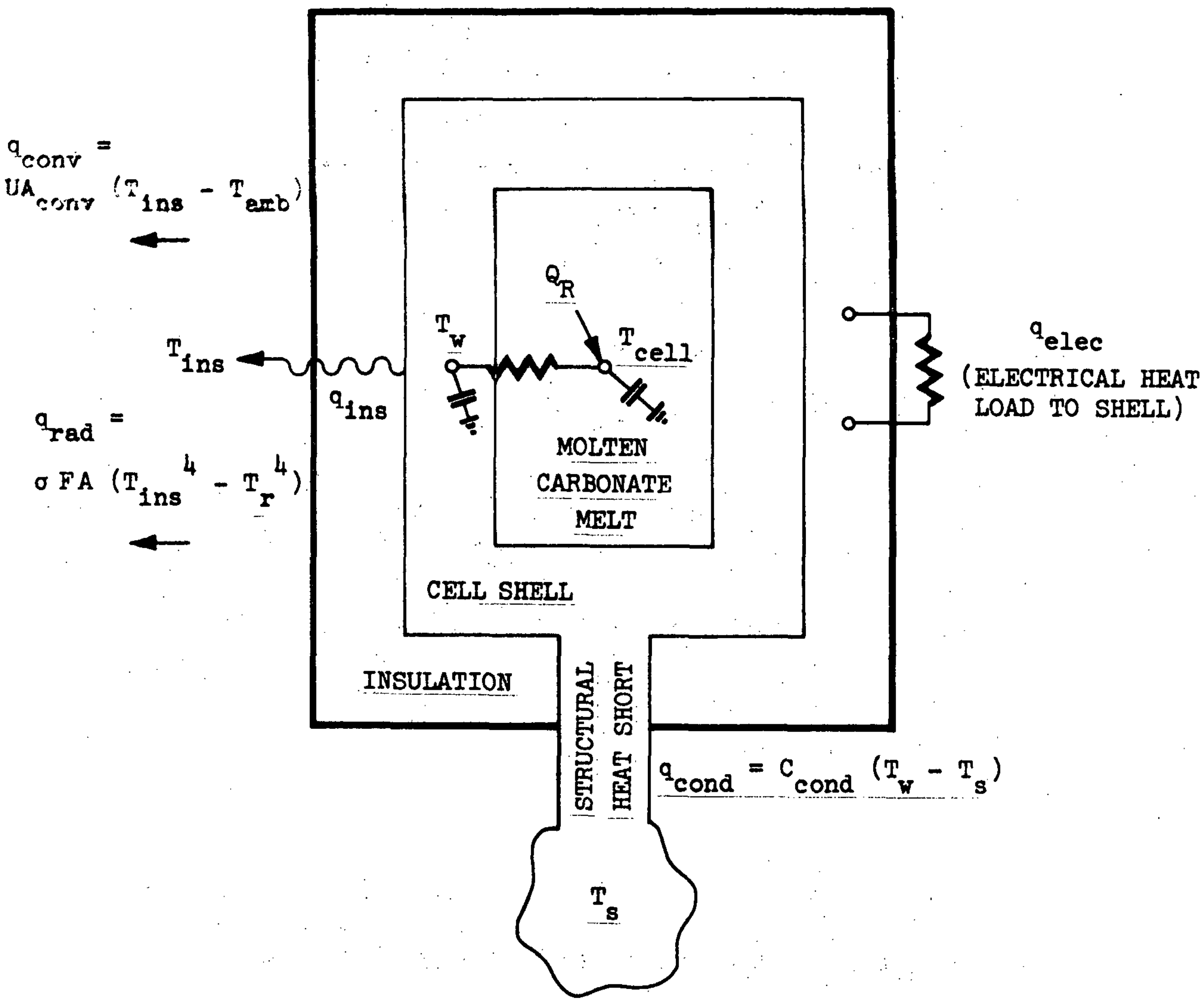
QLØSS = net heat loss to the surroundings by conduction, convection, and radiation (Btu/hr)

P = electrical energy dissipated in the cell due to inefficiency and joule heating = $(E_{cell} - 1.025) \times I \times 3.41$ (Btu/hr

QE = electrical energy dissipated by heaters (Btu/hr)

Table 1 - HEAT CAPACITY EQUATIONS FOR GASES INVOLVED IN MOLTEN CARBONATE CELL

O_2	$C_P = -187700.\ T^{-2} + 8.27 + .000258T \quad \frac{\text{cal}}{\text{g mole }^\circ\text{K}}$
N_2	$C_P = 6.50 + 0.00100T$
$H_2O_{(g)}$	$C_P = 8.22 + 0.00015T + 0.00000134T^2$
CO_2	$C_P = -195500.T^{-2} + 10.34 + 0.00274T^1$



$$q_{ins} = UA_{ins} (T_w - T_{ins})$$

$$= q_{conv} + q_{rad}$$

$$q_{surr} = q_{cond} + q_{conv} + q_{rad}$$

$$T_{cell} \simeq T_w$$

FIGURE 1. THERMAL MODEL FOR MOLTEN CARBONATE CELL

G = lumped thermal capacitance of cell (Btu/°F)

T_{cell}', T_{cell} = temperature of cell at time t + Δτ and time t, respectively (°F)

Δτ = computing time increment (hours)

Equation (12) is rewritten in the following form for solution by a trial and error technique.

$$PHI = - \frac{T_{cell}' - T_{cell}}{\Delta\tau} G - QL\emptyset SS + P + QE + \Delta H_T \qquad (13)$$

For a trial value of T_{cell}', QLØSS is calculated using subroutine QSURR. Equation (13) is solved for PHI. Subroutine ESTIM is then used to determine the value of T_{cell}' for which PHI equals 0. Convergence is satisfied when:

$$\left| \frac{PHI}{(P + QE + (NC_p)_R \ (T_{in})} \right| < \frac{R(72)}{100.}$$

4.0 Lower Level Subroutines and Functions

QSURR

ESTIM

5.0 References

1. Arnoldi, W. E.: "An Electrolytic Process for Carbon Dioxide Separation and Oxygen Reclamation." Atmosphere in Space Cabins and Closed Environments, Meredith Publishing Co., 1966, pp. 76-103.
2. Stein, P. J.: Research and Development Program for a Combined Carbon Dioxide Removal and Reduction System. Hamilton Standard Division, Contract No. NAS1-4154, Final Report - Phase I, Oct 1965.

SMGEN

Component Subroutine No. 27 - Steam Generator

1.0 Subroutine Description

The steam generator subroutine is used to supply superheated steam for use in various EC/LS subsystems. Options are available either to calculate the required heat input to meet a specified steam generation rate or to calculate the steam generation rate for a specified value of heat input. An option is available to simulate boilers with thermal energy being supplied by electrical current, a miscellaneous heat source such as a radioisotope, or a process heating fluid.

2.0 Subroutine Data

2.1 General Notes

1. The flow code for the primary side of this component is 1, 2, or 3. The component which provides the source of primary flow must have a flow code of 0 or 4.
2. The flow code for the secondary side of this component is 0 or 4. The component which provides the source of this secondary flow must also have a flow code of 0 or 4.
3. A primary flow source must be specified regardless of the instruction options (NSTR's) selected. The source will provide the inlet temperature and pressure for the water being vaporized. Outlet pressure of vapor is set equal to this value.
4. A secondary flow source must be specified only if the heat source for the generator is process heating fluid.
5. The generator is assumed to be perfectly insulated. Heat losses from the unit may be simulated with pipe or duct components up or downstream of the component.

2.2 Instruction Options

NSTR(1): Type of generator

= 0 Heat is supplied by electrical heating or other miscellaneous heat source

= 1 Heat is supplied by process heating fluid

NSTR(2): Method for performing calculations

= 0 Calculate steam generation rate for a specified process heating fluid flow rate, miscellaneous heat generation rate (or electrical energy dissipation), and liquid feed rate

= 1 Calculate heating fluid requirements or miscellaneous heat generation rate (or electrical energy dissipation) required to vaporize liquid water entering generator as primary flow (A(01)).

NSTR(3): Method for calculating heat exchanger performance

= 0 Effectiveness is input

= 1 Overall thermal conductance is input. Effectiveness is calculated assuming $\eta = 1 - e^{-NTU}$

where

$$NTU = \frac{UA}{(WC_p)_s}$$

UA = overall thermal conductance, $\frac{Btu}{hr\ °F}$

$(WC_p)_s$ = capacity flow rate for heating fluid (secondary flow)

2.3 Steady State V-Array Data

Reference Location	Description	Data Type
65	Not used	0
66	Desired degrees of superheat (°F)	I(R) if NSTR(2)=1

Reference Location	Description	Data Type
67	Temperature of saturated steam (°F)	0
68	Energy supplied by electrical or other miscellaneous heat source (watts	I(R) if NSTR(2)=0 and NSTR(1)=0
69	Heat exchanger effectiveness	I(R) if NSTR(1)=1 and NSTR(3)=0
70	Overall thermal conductance between steam (and water) and process heating fluid $\left(\mathrm{Btu}/\mathrm{hr}\ {}^\circ\mathrm{F}\right)$	I(R) if NSTR(1)=1 and NSTR(3)=1

3.0 Analytical Model Description

a. Required steam generation rate specified

$$Q = W_a \left(h_{g,o} - h_{1,i}\right)$$

where:

Q = required heat (Btu/hr)

$h_{1,i}$ = enthalpy of liquid entering generator (Btu/lb)

$h_{g,o}$ = enthalpy of superheated steam leaving (Btu/lb)

W_a = steam generation rate (lb/hr)

$$h_{1,i} = HF(T_1)$$

$$h_{g,o} = HG(T_2)$$

where:

T_1 = temperature of liquid water entering generator (°F)

T_2 = saturation temperature plus degrees superheat $\left[R(66)\right]$

HF and HG are built-in functions to determine enthalpy of liquid and vapor respectively.

for generator with electrical or miscellaneous heat source

$$R(68) = Q/3.41 \text{ (watts)}$$

for generator with heat supplied by process heating fluid, the flow is estimated as

$$W_b = {}^{Q}/_{C_{PB}\left(T_3 - T_4\right)}$$

where:

W_b = required flowrate of heating fluid (lb/hr)

C_{PB} = specific heat of heating fluid (Btu/lb°F)

T_3 = temperature of heating fluid entering generator (°F)

T_4 = temperature of saturated steam (°F)

b. Miscellaneous heating rate or process heating fluid flow rate specified. If miscellaneous heating (or electrical energy dissipation)

$$Q = R(68)$$

if heat supplied by process heating fluid

$$Q = \eta W_b C_{PB}\left(T_3 - T_1\right)$$

where:

η = heat exchanger effectiveness

(1) if $Q > W_a \left(h_{s,o} - h_{1,i}\right)$

$$T_{out} = T_{sat} = \frac{Q - W_a\ (h_{s,o} - h_{1,i})}{W_a C_{PA}}$$

where:

Q = specified heating rate (Btu/hr)

W_a = steam generation rate (lb/hr)

$h_{s,o}$ = enthalpy of saturated steam (Btu/lb)

$h_{1,i}$ = enthalpy of liquid water entering generator (Btu/lb)

C_{PA} = specific heat of steam (Btu/lb°F)

T_{out} = temperature of steam leaving (°F)

T_{sat} = temperature of saturated steam (°F)

(2) if $Q < W_a \left(h_{g,o} - h_{1,i}\right)$

$$h_{t,o} = \frac{Q}{W_a} + h_{1,i}$$

$$T_{out} = T_1 + \frac{Q}{(W_a)\ (C_{PW})} \qquad \underline{\text{if } h_{t,o} < h_{1,o}}$$

where:

T_1 = temperature of liquid water entering generator (°F)

C_{PW} = specific heat if liquid water $\left(\frac{Btu}{lb\,°F}\right) = 1.0$

$h_{1,o}$ = enthalpy of liquid water at saturation temperature $\left(\frac{Btu}{lb}\right)$

$h_{t,o}$ = enthalpy of mixture of vapor and liquid leaving generator(Btu/lb) or

$T_{out} = T_{sat}$ if $h_{t,o} > h_{1,o}$

for this condition

$W_1 = (1-x)W_a$ = liquid water leaving (lb/hr)

$W_v = XW_a$ = vapor leaving (lb/hr)

$X = \frac{h_{t,o} - h_{1,o}}{h_{g,o} - h_{1,o}}$ = fraction vapor in stream leaving generator

4.0 Lower Level Subroutines Required

HG

TSAT

HF

5.0 References

None

S0LEL

Component Subroutine No. 51 - Solid Electrolyte Cells

1.0 Subroutine Description

This subroutine is used to simulate the reduction of CO_2 to O_2 in a solid electrolyte cell unit. This method of CO_2 reduction differs from other potential concepts in that the feed gas need not be dry. CO_2 and H_2O are both electrochemically decomposed.

The physical geometry of a unit is described in general terms. That is, the unit is assumed to be comprised of a number of parallel modules to which the flow and current divide equally. Each module is comprised of a number of cell stacks. The cell stacks are assumed to be connected in parallel electrically. Module flow is assumed to divide equally between the stacks. Stack cells are assumed to be connected in series.

For heat transfer purposes, each module is treated as a single lumped mass. Heat losses to the ambient air and structure may be simulated by specifying appropriate input data.

2.0 Subroutine Data

2.1 General Notes

1. A primary source flow must be specified to provide an inlet gas flow. The primary side flow code must be 3. The flow constituents in the source of flow must be compatible with those for the component.
2. A flow code of 2 or 3 must be specified for the secondary side of this component. The secondary flowout of this component will be composed of the oxygen gas generated in the cell.
3. The gaseous feed for the primary side of the component is assumed to be composed of CO_2, H_2O, CO, and H_2. The CO may

enter as recycle flow from the disproportionator reactor (CARDP) used to form CO_2 from CO generated in the solid electrolyte cells. Normally, H_2 generated in the cell will be separated out through a semi-permeable membrane. Small amounts, however, may enter as recycle flow. Oxygen and nitrogen should be present only in negligible amounts. H_2 and CO are assumed to enter as special flows 2 and 3, respectively.

4. The unit is assumed to be comprised of a number of parallel modules. Each module is comprised of a number of cell stacks which are also connected in parallel. Flow is assumed to divide equally between the stacks. Each stack is made up of a number of cells connected electrically in series. Flow divides equally among the cells. Figure 1 illustrates how two different concepts may be modeled.

2.2 Instruction Options

NSTR(1): Specifies method for determining cell voltage

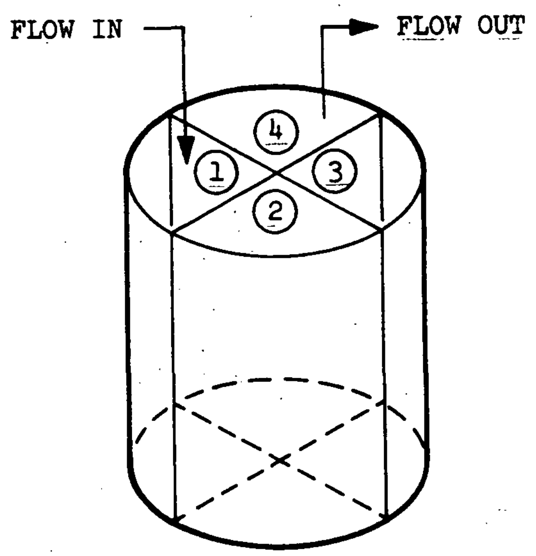
= 0 Cell voltage is calculated from the theoretical cell voltage and power efficiency specified in R(76).

= 1 Cell voltage is determined by interpolating a table of values of cell voltage versus current density (amps/ft^2) and cell temperature (°F)

NSTR(2): Specifies method for determining electrolysis current

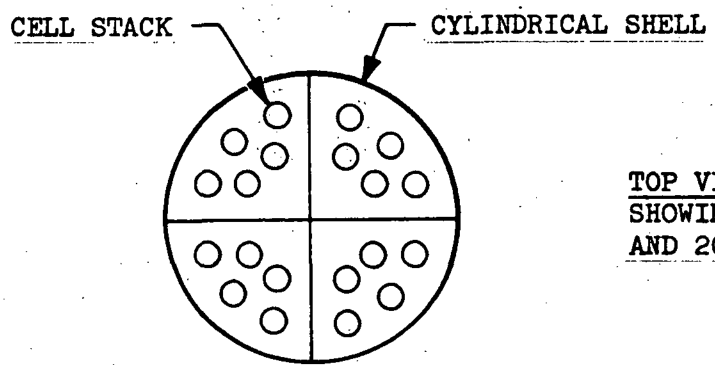
= 0 Total current to unit is a constant value input in R(67). Electrolysis current is calculated from O_2 current efficiency specified in R(72).

= 1 Cell electrolysis current is calculated from O_2 current efficiency and the constant value of CO_2 and H_2O conversion $\frac{lb_{in} - lb_{out}}{lb_{in}}$ specified in R(70) and R(71).

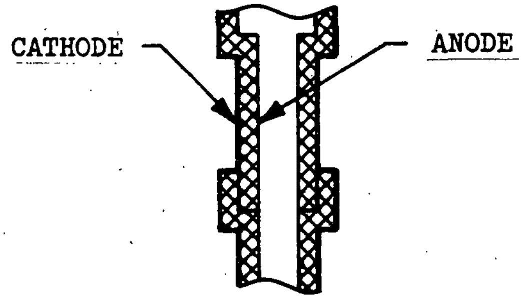


1 MODULE
20 STACKS
7 CELLS/STACK

BAFFLES DIVIDE CYLINDER INTO 4 COMPARTMENTS. TOTAL FLOW FLOWS FROM ONE COMPARTMENT INTO NEXT.



TOP VIEW
SHOWING 4 COMPARTMENTS
AND 20 CELL STACKS



SIDE VIEW
OF BELL AND SPIGOT
CELL CROSS SECTION
7 CELLS/STACK

FIGURE 1a DETAILS OF BELL AND SPIGOT CONCEPT

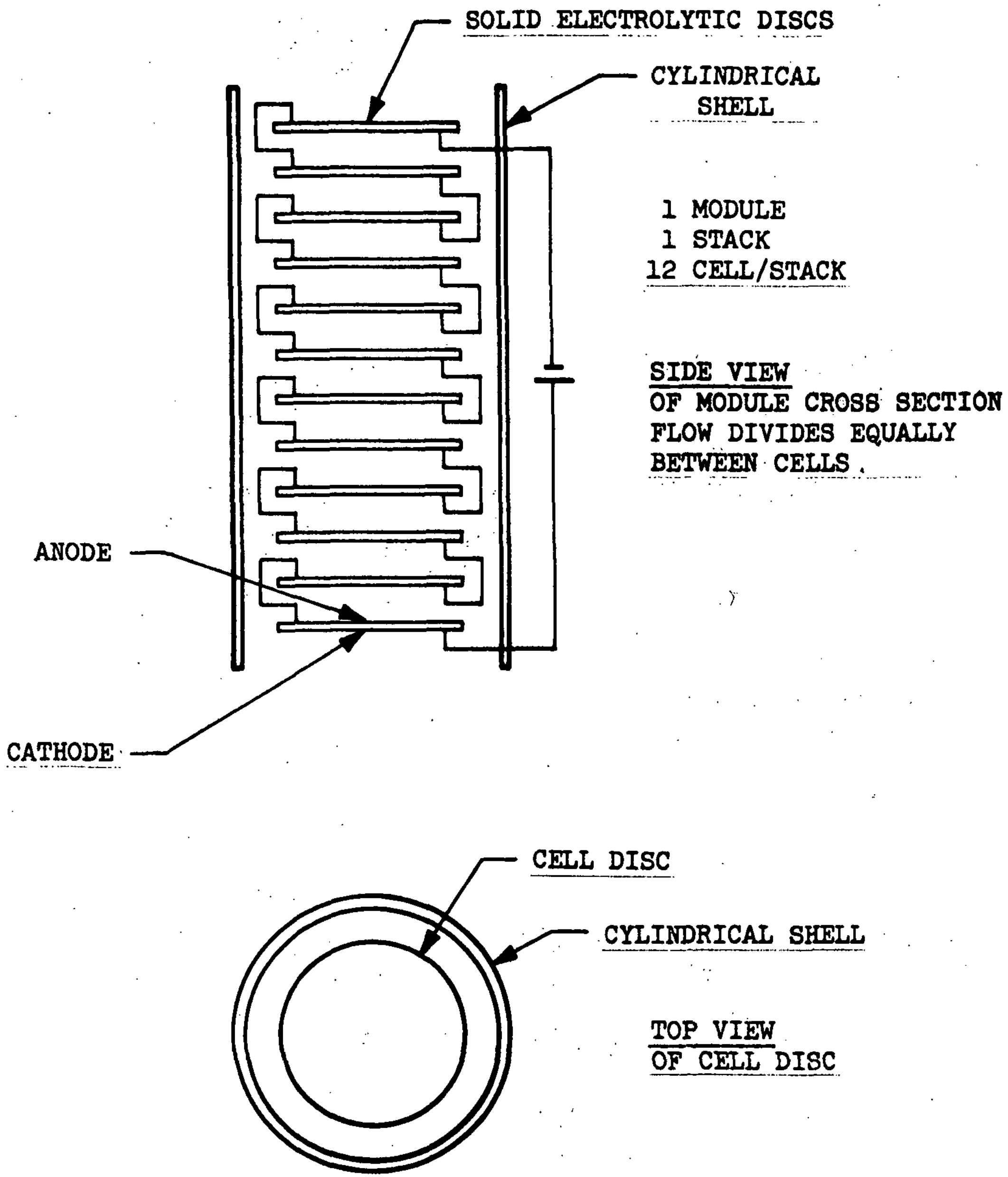


FIGURE 1b DETAILS OF DISC CONCEPT

2.3 Heat Loss V-Array Data

Reference Location	Description	Data Type
51	Temperature of a module shell (°F)	0
52	Effective thermal conductance from module shell to surroundings (Btu/hr°F)	0
53	Total heat loss from module to surroundings (Btu/hr) R(53)=R(56)+R(59)+R(62)	0
54	Ambient gas temperature (°F)	I(R)
55	Thermal conductance between surface of module insulation and ambient gas (Btu/hr-°F)	I(R)
56	Convective heat loss to ambient gas (Btu/hr) from a module	0
57	Ambient wall temperature (°F)	I(R)
58	Module thermal radiation FA from surface of insulation to ambient wall (ft^2)	I(R)
59	Radiative heat loss from a module to ambient wall (Btu/hr)	0
60	Structure temperature (°F)	I(R)
61	Conductance ($^{kA}/\Delta x$) between module shell and structure (Btu/hr	I(R)
62	Conductive heat loss to the structure (Btu/hr)	0
63	Insulation surface temperature (°F)	0
64	Conductance ($\frac{kA}{\Delta x}$) between module shell and outer surface of insulation	I(0)

2.4 Steady State K-Array Data

Reference Location	Description	Data Type
16	Number of cells/stack	I(R)
17	Number of stacks/module	I(R)
18	Number of modules/unit	I(R)
19	Table number for cell voltage (volts) as a function of current density (amps/ft^2) and temperature (°F)	I(0)

2.5 Steady State V-Array Data

Reference Location	Description	Data Type
65	Heat dissipated in a module by electrical heater (Btu/hr)	I(0)
66	Heat dissipated in a module due to current and voltage inefficiency (Btu/hr)	0
67	Total current to <u>unit</u> (amps)	I(R) if NSTR(2)=0
68	Total electrolysis current to a module (amps)	0
69	Current density (amps/ft^2)	0
70	CO_2 conversion (fraction)	I(R) if NSTR(2)=1
71	H_2O conversion (fraction)	I(R) if NSTR(2)=1
72	Overall O_2 current efficiency (fraction)	I(R)
73	CO current efficiency (equals 1.0-R(74)	0
74	H_2 current efficiency (fraction)	I(R)
75	Cell voltage (volts)	0
76	Voltage efficiency, E_{thr}/E_{act}, (fraction)	I(R) if NSTR(1)=0
77	Electrode area for cell (ft^2)	I(R) if NSTR(1)=1
78	Previous trial value for PHI (Btu/hr)*	0
79	Previous trial value for T_{MOD} (°F)*	0
80	Convergence tolerance for calculating cell temperature (percent)	0

---

* These quantities are used in the trial and error method used for determining module temperature. The technique is described in section 3.0.

2.6 Transient V-Array Data

Reference Location	Description	Data Type
R(81)	Total module thermal capacitance (Btu/°F	I(R)
R(82)	Initial temperature at time t (°F)	I(R)

3.0 Analytical Model Description

CO_2 is reduced in this process by the following electrochemical reactions:

at cathode:

$$2CO_2 + 4e^- \longrightarrow 2CO + 2O^= \quad (1)$$

at anode:

$$2O^= \longrightarrow O_2 + 4e^- \quad (2)$$

or a net reaction of

$$2CO_2 \longrightarrow 2CO + O_2 \quad (3)$$

Simultaneously with the above reactions

H_2O is electrolyzed as follows:

at cathode:

$$2H_2O + 4e^- \longrightarrow 2H_2 + 2O^= \quad (4)$$

at anode:

$$2O^= \longrightarrow O_2 + 4e^- \quad (5)$$

or net reaction of

$$2H_2O \longrightarrow 2H_2 + O_2 \quad (6)$$

By Faraday's law, the total amount of oxygen generated by reactions (3) and (4) will be

$$W_{O_2} = I_e/1508 \text{ (lb/hr)} \quad (7)$$

where:

I_e = electrolysis current (amps)

The amounts of CO_2 and H_2O reacted (or CO and H_2 formed) are more difficult to predict analytically. A simplified approach is used using experimentally determined values for current efficiencies for CO and H_2 formation

$$N_{CO} = \frac{M_{CO} \times 24100}{I_e} \qquad (8)$$

$$N_{H_2} = \frac{M_{H_2} \times 24100}{I_e} \qquad (9)$$

where:

M_{CO} = lb moles CO formed (lb moles/hr)

M_{H_2} = lb moles H_2 formed (lb moles/hr)

I_e = electrolysis current (amps)

$N_{CO} + N_{H_2} = 1.0$

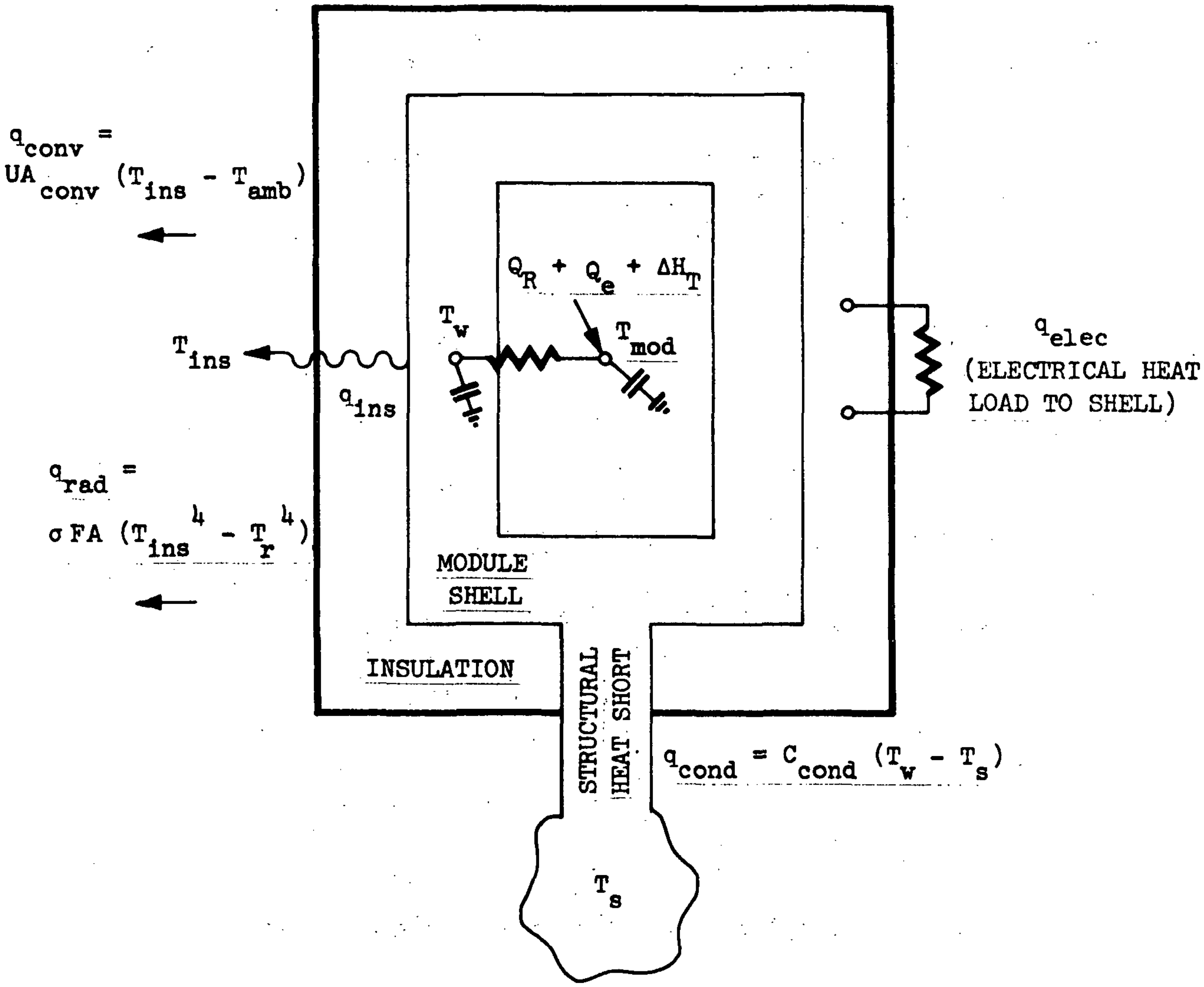
The electrolysis current generally will be less than the total current due to miscellaneous shunt losses in the cells. The O_2 current efficiency thus is defined as the following:

$$N_{O_2} = \frac{I_e}{I_t} \qquad (10)$$

where:

I_t = total cell current (amps)

The cell module is treated as a single lumped mass for transient heat transfer calculations. A heat balance is performed taking into account losses to the ambient (by conduction, radiation, and convection), electrical energy dissipated as heat, energy supplied by an electrical heater, and the net enthalpy change of products and reactants, and the heat of reaction for equations (3) and (6). Figure 2 illustrates the thermal model used in this subroutine.



$$q_{ins} = UA_{ins} (T_w - T_{ins})$$
$$= q_{conv} + q_{rad}$$

$$q_{surr} = q_{cond} + q_{conv} + q_{rad}$$

$$T_{mod} \simeq T_w$$

FIGURE 2 THERMAL MODEL FOR SOLID ELECTROLYTE CELL MODULE

The net enthalpy added by the influx and efflux of reactants and products, respectively, and the heat absorbed by chemical reaction is included in the heat balance mentioned previously. Since the enthalpy change is independent of the thermodynamic path chosen, the net enthalpy added to the module is as follows:

$$\Delta H_T = \Delta H_R - \Delta H_P - \Delta H_{1,TO} - \Delta H_{2,\,TO} \tag{11}$$

when:

$\Delta H_{1,TO}$ = heat of reaction for decomposition of CO_2 at 77°F (Btu/hr)

$\Delta H_{2,TO}$ = heat of reaction for decomposition of H_2O at 77°F (Btu/hr)

ΔH_R and ΔH_P are the integrated enthalpy changes for the reactants and products, respectively, from the inlet and outlet temperatures to the standard state for the heat of reaction (77°F). The integrated enthalpy change for each species is calculated by the following equation:

$$\Delta H_i = N_i \int_{T_o}^{T} \left(aT^{-2} + bT^{-1} + cT^{\circ} + dT^{1} + eT^{2} \right) dT \tag{12}$$

where:

N_i = flow rate (lb/hr)

ΔH_i = enthalpy change for constituent i between temperature T and T_o

a, b, c, d = experimentally determined coefficients for heat capacity as a function of temperature. The values of these constants for the reactant and product constituents are given in Table I.

The theoretical decomposition voltage for CO_2 and H_2O are both fairly close. At 850°C they are as follows:

$$E_{H_2O} = 1.102 \text{ volts}$$

$$E_{CO_2} = 0.956 \text{ volts}$$

The actual cell voltage has been found to be approximately 1.8 volts. The subroutine has an option for entering tabular data for cell voltage as a function of current density and cell temperature. Alternatively, the cell may be calculated from the cell efficiency

$$E_{cell} = \frac{1.102}{N_{cell}} \qquad (13)$$

For heat transfer calculations, the amount of electrical energy dissipated due to current and voltage inefficiency is as follows:

$$Q_e = \left[E_{cell}\ I_t - 1.102\ I_e \atop \text{Btu/hr)} \right] \times 3.41 \qquad (14)$$

The heat balance for the module temperature is given below:

$$\frac{T_{MOD}' - T_{MOD}}{\Delta\tau} G = -Q_{AM} + Q_e + Q_H + \Delta H_T \qquad (15)$$

where:

Q_{AM} = net heat loss to the surroundings by conduction, convection, and ratiation (Btu/hr)

Q_e = electrical energy dissipated in the cells due to inefficiency and Joule heating

Q_H = energy dissipated by electrical heater (Btu/hr)

ΔH_T = net enthalpy added to module by reactants and products and heat of reaction (Btu/hr)

G = module lumped thermal capacitance (Btu/°F)

Table I - CONSTANTS FOR HEAT CAPACITY EQUATIONS

$$C_P = a/_{T}2 + b/_{T} + c + dT^1 + eT^2 \qquad \frac{\text{cal}}{\text{g mole °K}}$$

	a	b	c	d	e
$O_{2(g)}$	-187700.	0.	8.27	.000258	0.
$H_2O(g)$	0.	0.	8.22	.00015	.00000134
CO_2	-195500.	0.	10.34	.00274	0.
C (graphile)	0.	0.	2.673	.002617	-116900.
H_2	0.	0.	6.62	.00081	0.
CO	0.	0.	6.60	.00120	0.

Equation (15) is rewritten in the following form for solution by a trial and error procedure.

$$PHI = -\frac{T_{MOD}' - T_{MOD}}{\Delta\tau} G - Q_{AM} + Q_e + Q_H + \Delta H_T \qquad (16)$$

For a trial value of T_{MOD}', Q_{AM} is calculated using subroutine QSURR. Equation (16) is then solved for PHI. Subroutine ESTIM is then used to determine the value of T_{MOD}' for which PHI equals 0. Convergence is satisfied when:

$$\left| \frac{PHI}{\Delta H_R + Q_e + Q_H} \right| < \frac{R(80)}{100}$$

4.0 Lower Level Subroutines and Functions

QSURR

ESTIM

5.0 References

1. Weissbart, J., Smart, Wydeven, "Design and Performance of a Solid Electrolyte Oxygen Generator Test Module," ASME Paper 71-Av-8.
2. Weissbart, et al, "Development of CO_2-H_2O Solid Oxide Electrolyte Electrolysis System"--2nd Annual Report - May 1970. NAS2-4848.
3. Elikan, L., Morris, Saunders, "180-Day Life Test of Solid Electrolyte System for Oxygen Regeneration," ASME Paper 71-Av-32.
4. Elikan, L., Morris, Wu , "Development of a Solid Electrolyte System for Oxygen Reclamation," NAS1-8896.
5. J. Weissbart and W. H. Smart, "Study of Electrolytic Dissociation of CO_2-H_2O Using a Solid Oxide Electrolyte," Feb 1967, NASA CR-680.

VACPMP

Component Subroutine No. 28 - Vacuum Pump

1.0 Subroutine Description

The performance of a vacuum pump may be simulated with this component. Depending on the options selected by the program user, table data may be interpolated for electrical input power and flow as a function of inlet and outlet pressure. Alternately, the work for compression may be predicted from the equation for an isentropic compression. The flow may be calculated from the equation for a single stage reciprocating compressor. The shaft and electrical input power are then calculated from the isentropic work using specified values for aerodynamic and motor efficiency.

Since the performance of this component is highly sensitive to variations in upstream and downstream pressures, a small subloop should be made for the affected components. For example, for a sorption bed being desorbed by heat and vacuum with the desorbed gas being pumped to an accumulator, a subloop should be set up with these components. The computing interval required for these components generally will be smaller than that required for the complete EC/LS system. Thus, GP0LY logic should be prepared to set up to allow iteration of the three components until the number of iterations times the loop computing interval equals the system computing interval.

2.0 Subroutine Data

2.1 General Notes

1. A primary flow source must be specified to provide an inlet gas flow.
2. The primary side flow code must be 1, 2, or 3.
3. The flow constituents for the source of flow must be compatible with those of the component.
4. The discharge pressure for the compressor must be input into R(75). The value for this parameter should be calculated by

appropriate GP0LY logic. Numerically, it should equal the pressure of the accumulator into which the gas is being pumped plus the line and other miscellaneous losses between the pump and accumulator.

2.2 Instruction Options

NSTR(1): Specifies method for determining flow

= 0 Set flow equal to inlet flow A(01)

= 1 Interpolate for flow as a function of P_{o/P_i}, and T_i

where:

P_i = inlet pressure (psia)

P_o = outlet pressure (psia)

T_i = inlet temperature (°F)

= 2 Calculate flow from built-in equations for reciprocating polytropic compression

NSTR(2): Specifies method for determining electrical input power

= 0 Constant value entered in R(69)

= 1 Determine input power from equation for isentropic compression

= 2 Interpolate for flow as a function of P_{o/P_i}, T_i

NSTR(3): Option for overriding calculations for flow during <u>steady state</u>

= 1 Set flow equal to inlet flow A(01)

= 2 Set flow equal to outlet flow R(01)

2.3 Heat Loss V-Array Data

Reference Location	Description	Data Type
51	Heat lost to ambient (Btu/hr)	0

2.4 Steady State K-Array Data

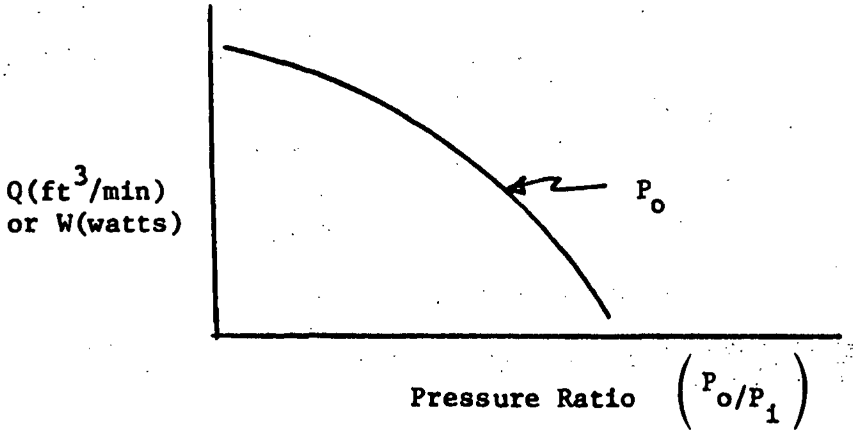
Reference Location	Description	Data Type
16	Table number for compressor flow (cfm) (based on inlet density) as a function of P_o/P_i, T_i	I(R) if NSTR(1)=0
17	Table number for compressor input power (watts) as a function of P_o/P_i, T_i	I(R) if NSTR(2)=2

2.5 Steady State V-Array Data

Reference Location	Description	Data Type
65	Total heat added to gas stream (Btu/hr)	0
66	Motor efficiency (dimensionless)	I(R)
67	Aerodynamic efficiency (dimensionless)	I(R)
68	Power required for compression (watts)	0
69	Total electrical input power (watts)	I(R) if NSTR(2)=0
70	Heat dissipated due to motor inefficiency (watts)	0
71	Fraction of heat dissipation, R(70), which is lost to ambient. 0 1	I(R)
72	Compressor piston displacement (ft^3/min)	I(R) if NSTR(1)=1
73	Clearance factor (dimensionless)	I(R) if NSTR(1)=1
74	Polytropic exponent (equals $\gamma = \frac{C_p}{C_v}$ for ideal gas)	I(R)
75	Discharge pressure (psia)	I(R)

3.0 Analytical Model Description

The vacuum pump flow and electrical input power may be determined by interpolation of bi-variant table data describing the pump performance. For example



where

$$\dot{m} = Q/v$$

Alternatively, the flow can be calculated from the equation given below for a single stage reciprocating compression

$$m = \left[1 + C - C\left(\frac{P_o}{P_i}\right)^{1/n}\right] \frac{P.D}{v_i}$$

where

$\dot{m}$ = flow rate (lb/min)

$C \equiv$ clearance factor = $\frac{\text{Clear Volume}}{\text{Displacement}}$

$P.D$ = piston displacement (ft^3/min)

v_i = specific volume of gas entering (ft^3/lb)

P_o = outlet pressure (lb/ft^2)

P_i = inlet pressure (lb/ft^2)

n = polytropic exponent

The isentropic work for this compression is given by

$$W_{isen} = \frac{n}{n-1} \; P_i v_i \left[\left(\frac{P_o}{P_i} \right)^{\frac{n-1}{n}} - 1 \right] \qquad \frac{\text{ft-lb}}{\text{lb}_m}$$

The shaft work required is calculated as follows:

$$W_s = \frac{W_{isen}}{N_{aero}}$$

where:

N_{aero} = aerodynamic efficiency

The electrical input power is calculated as follows:

$$W_{IP} = \frac{W_s}{N_m}$$

where

$N_m \equiv$ motor efficiency

The total heat dissipated due to inefficiency in the motor is thus

$$Q = W_{IP} \, (1 - N_m)$$

The fraction of this heat which is dissipated to the surrounding (the remainder being dissipated into the gas being pumped) is specified as input data.

The total heat being dissipated into the gas being pumped is thus

$$Q_t = \left[W_s + \left(1. - F\right) W_{IP} \left(1. - N_m\right) \right] 3.41$$

when

F = fraction of heat dissipated to surroundings

The temperature rise for the gas due to compression plus inefficiency is thus

$$T_{out} = T_{in} + \frac{Q_t}{\dot{W} C_p}$$

4.0 Lower Level Subroutines and Functions

None.

5.0 References

None.

APPENDIX B

NEW UTILITY OR SPECIAL PURPOSE SUBROUTINES

C0ABS

1.0 Purpose

This subroutine computes transient performance of sorbing or purge desorbing packed resin beds.

2.0 Use

This routine is used by component subroutine C0S0RP to simulate absorption or adsorption processes.

3.0 Calling Sequence

Call C0ABS

4.0 Output

The computed output for this routine is stored in the R array for C0S0RP. These output are discussed in section 2.8 of C0S0RP.

5.0 Method

The equations and assumptions used in preparing this routine are discussed in section 3.2.1 of C0S0RP.

CO2CP

1.0 Purpose

Subroutine CO2CP computes the effective c_p, denoted as $\bar{c}_p$, for primary and/or secondary flow to account for the precipitation of CO_2 in the heat exchanger. The subroutine computes the amount of CO_2 removed due to the precipitation process which can occur in the gas stream. The effective value of C_p accounts for the effects of precipitation and yields better results in temperature in heat exchanger performance calculations.

2.0 Use

2.1 The subroutine is called by ANYHX during steady state solutions when precipitation of CO_2 can occur; that is, NSTR(9) is set to 1.

2.2 The subroutine is called twice by ANYHX (NSTR(9) = 1) during transient conditions when a steady state solution is required. The first call is used in obtaining $\bar{c}_p$ based on inlet and outlet temperatures at the start of the time step. The second call is used to obtain updated values for $\bar{c}_p$ following the calculation of new outlet temperatures, for the end of the time step, in ANYHXT.

3.0 Calling Sequence

CALL CO2CP

4.0 Output

Data computed in this subroutine are stored in the R-array for ANYHX. These data are discussed below:

R(12) and/or R(31), CO_2 outflow, lb/hr
R(72) and/or R(73), Effective specific heats
R(68) and/or R(69), Precipitation rate

The effective specific heats are named XCP(1) and XCP(2) for primary and secondary streams in the heat exchanger common block/CANYXH/.

5.0 Method

When ANYHX calls CO_2CP precipitation of CO_2 is anticipated in the heat exchanger. The subroutine initially sets up functions which compute enthalpies and specific heats for solid and vapor and implemented into the program as follows:

$$c_{p_g}(T) = \frac{8.71 + .0066\,T - 22 \times 10^{-7}\,T^2}{44.0} \tag{1}$$

(Reference 1)

$$c_{p_s}(T) = .397 + .00115\,T \tag{2}$$

(Reference 2)

$$h_g(T) = 136. + T\,(c_p(T) + 69.2\,c_p(T_s) \tag{3}$$

$$h_s(T) = T\,c_{p_s}(T) + 40.0\,c_{p_s}(-40) - 88.7 \tag{4}$$

(Reference 3)

where,

$c_{p_s}(T)$ = Specific heat of solid CO_2 at temperature T, Btu/lb-°F

$c_{p_g}(T)$ = Specific heat of CO_2 vapor at temperature T, Btu/lb-°F

$h_g(T)$ = Enthalpy of CO_2 vapor at temperature T, Btu.

$h_s(T)$ = Enthalpy of CO_2 solid at temperature T, Btu

T = Outlet temperature of cabin air, °C

T_s = Temperature at which CO_2 changes phase, $-56.2°C = -69.2°F$

The saturation pressure and max allowable CO_2 flowrate is determined from the following relationship:

$$\text{Log}_{10}\ (\text{PCO2}) = \frac{-1275.6}{\text{TK}} + .00683\ \text{TK} + 8.307\ (\text{TK} > 150.) \qquad (5)$$

$$\text{Log}_{10}\ (\text{PCO2}) = \frac{-1352.6}{\text{TK}} + 9.83\ (\text{TK} < 150.) \qquad (6)$$

(Reference 4)

where,

PCO2 = CO_2 saturation pressure at temperature TK, mmHg

TK = Heat exchanger outlet temperature, °K.

From saturation pressure of CO_2, maximum CO_2 flowrate is computed. If the inlet CO_2 flow is greater than maximum CO_2 flow allowable we assure the difference to percipitate out, thus modifying our effective specific heat value. The effective specific heat is then computed from the following relationship:

$$\bar{c}_p = \frac{(\dot{w}_{nc} * c_{p_{nc}} * T_i + w_{CO_2} * h_g\ (T_i)\ ) - (\dot{w}_{nc} * c_{p_{nc}}\ T_o + w_{CO_2} * h_g\ (T_o) + w_{c,s} * h_s\ (T_o)\ )}{\dot{w}_{nc} * (T_i - T_o)} =$$

where:

$\dot{w}_{nc}$ = Non-condensable flowrate, lbs/hr

$C_{p_{nc}}$ = Specific heat of non-condensables, Btu/lb-°F

T_i = Air inlet temperature, °F

T_o = Air outlet temperature, °F

$\dot{w}_{CO_2}$ = CO_2 flowrate, lb/hr

h_g = Gaseous CO_2 enthalpy, Btu/lb

h_s = Solid CO_2 enthalpy, Btu/lb

$\bar{c}_p$ = Effective specific heat, Btu/lb-°F

$\dot{w}_{c_s}$ = CO_2 freezing rate, lb/hr

6.0 References

1. International Critical Tables Vol. V, p. 83. McGraw-Hill Book Co., New York, New York 1929

2. International Critical Tables Vol V, p. 95. McGraw Hill Book Co., New York, New York 1929.

3. ASRAE Guide and Data Book Fundamentals and Equipment, p. 342. American Society of Heating Refrigerating and Air Conditioning Engineers, Inc., New York, New York, 1965/1966.

4. International Critical Tables, Vol. III, p. 207. McGraw Hill Book Co., New York, New York, 1929.

SDESRP

1. 0 Purpose

This subroutine computes transient performance of steam desorbed packed resin beds.

2.0 Use

This routine is used by component subroutine CØSØRP to simulate steam desorption processes.

3.0 Calling Sequence

Call SDESRP

4.0 Output

The computed output for this routine is stored in the R array for CØSØRP. The output are discussed in section 2.8 of CØSØRP.

5.0 Method

The equations and assumptions used in preparing this routine are discussed in section 3.2.2 of CØSØRP.

SSSØR

1.0 Purpose

This subroutine computes the steady state performance of sorption beds.

2.0 Use

The routine is used by component subroutine CØSØRP to calculate the steady state absorption/adsorption, purge desorption, thermal vacuum and steam desorption of packed resin beds.

3.0 Calling Sequence

Call SSSØR

4.0 Output

The computed output of the routine is stored in the R-array for CØSØRP. These output are discussed in section 2.5 of CØSØRP.

5.0 Method

The methods used for this routine are discussed in sections 3.1.1 3.1.2 and 3.1.3 of CØSØRP.

PØLFT

1.0 Purpose

The purpose of this routine is to perform parabolic interpolation of three pairs of values of independent and dependent variables.

2.0 Use

This routine is used by subroutines CØABS, SDESRP, VACDSP, and SSSØR (lower level subroutines for CØSØRP) to interpolate for the absorption bed CO_2 equilibrium partial pressure at a specified value of CO_2 bed loading and three values of water bed loading. However, the routine is general in nature and can be used to interpolate between any three pairs of values of independent and dependent variables.

3.0 Calling Sequence

Z = POLFT (Y, X, XVALUE)

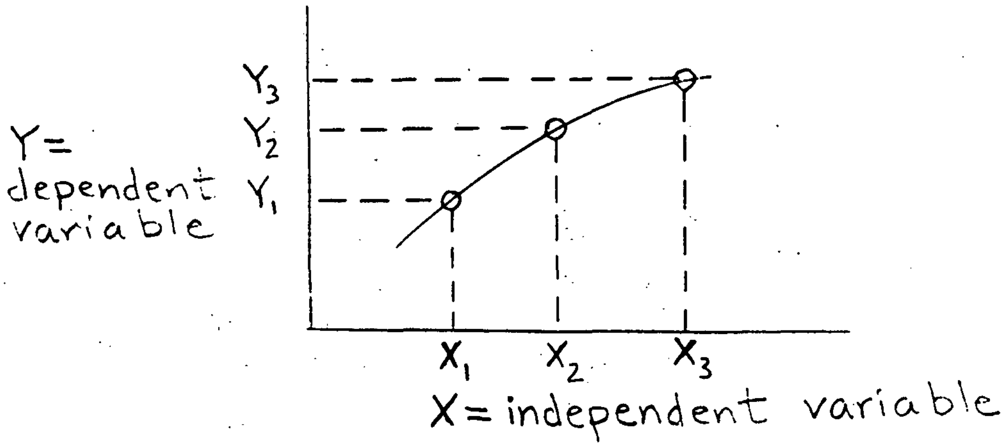
Function Value or Argument	Type	I/O	Description
POLFT ( )	R	O	interpolated value of dependent variable
Y	R	I	array of 3 values of dependent variables
X	R	I	array of 3 values of independent variables
X VALUE	R	I	value of independent variable

example: Z = POLFT (PP(1), VAR(1), RX(J+06))

4.0 Output

Returns a value for PØLFT ( ) as described above.

5.0 Method



$$y = a + bX + cX^2$$

where:

$$a = y_1 - X_1 b - X_1^2 c$$

$$b = \frac{(y_1 - y_2) - (X_1^2 - X_2^2)\, c}{(X_1 - X_2)}$$

$$c = \frac{(y_1 - y_2) - \left| \frac{X_1 - X_2}{X_2 - X_3} \right| (y_2 - y_3)}{\left[(X_1^2 - X_2^2) - \left(\frac{X_1 - X_2)}{(X_2 - X_3} \right) (X_2^2 - X_3^2) \right]}$$

VACDSP

1.0 Purpose

This subroutine computes transient performance of sorption beds which are desorbed by the combined effects of heat and vacuum.

2.0 Use

This routine is used by component subroutine C0S0RP to simulate thermal/vacuum desorption.

3.0 Calling Sequence

Call VACDSP

4.0 Output

The computed output for this routine is stored in the R array for C0S0RP. These outputs are discussed in Section 2.8 of C0S0RP.

5.0 Method

The equations and assumptions used in preparing this routine are discussed in Section 3.2.3 of C0S0RP.

6.0 Lower Level Subroutines

VLC02

1.0 Purpose

This routine is used to calculate the equilibrium partial pressure of CO_2 over IR-45 solid amine resin for specified values of CO_2 and H_2O bed loading and bed temperature.

2.0 Use

This function is used by subroutines C0ABS, SDESRP, VACDSP, and SSS0R (lower leve subroutines for component subroutine COS0RP). The partial pressure of CO_2 is used to determine the mass transfer rate of CO_2 from the carrier gas to the bed.

3.0 Calling Sequence

Z = VLC02(S,W,T)

Function Value or Argument	Type	I/O	Description
VLC02 ( )	R	O	Equilibrium partial pressure (lb/in^2)
S	R	I	Bed CO_2 loading $\frac{lb\ CO_2}{lb_{dry\ resin}}$
W	R	I	Bed H_2O loading $\frac{lb_{H_2O}}{lb\ dry\ resin}$
T	R	I	Temperature (°F) of bed.

example:

Z = VLC02 (RX(J+02), RX (J+04), RX(J+06))

4.0 Output

Returns a value of VLC02 (   ) as described above.

5.0 Method

The equilibrium partial pressure of CO_2 is calculated by equations (1), (2), and (3). The assumptions and methods used in the development of equation (1) were presented in reference 1. The equation is based on data reported in references (2) and (3). Equation (2) was determined from a least squares fit if data reported in reference 4. equation (3) is based on a technique reported in reference (5).

$$P^{*}_{CO_2,77} = \left[\frac{0.587}{\ln(.24 + 16.7W) - \ln(100S)}\right]^2 \frac{14.7}{760.} \qquad (1)$$

$$P^{Sat}_{CO_2,T} = e^{X} \qquad (2)$$

Where:

$$X = 14.205635 - 4274.967\,\frac{1}{T} + 172599.27\,\frac{1}{T}^{2}$$

$$P^{*}_{CO_2,T} = P^{Sat}_{CO_2,T}\left[\frac{P^{*}_{CO_2,77}}{P^{Sat}_{CO_2,77}}\right]^{539/T} \qquad (3)$$

where:

$P^{*}_{CO_2,77}$ = equilibrium partial pressure of CO_2 at 77°F (psia)

$P_{CO_2,T}$ = saturation pressure for CO_2 at temperature T (psia)

$P^{*}_{CO_2,T}$ = equilibrium partial pressure of CO_2 at temperature T (psia)

W, S, T = previously defined

6.0 References

1. 2nd Monthly Progress Report, Attachment 1, page 11 thru 13, Contract No. NAS9-12076, Advanced ETC/LSS Computerized Analytical Models, September 16, 1971.

2. MSA Research Corporation: Development of System Design Information For Carbon Dioxide Using an Amine Type Sorber NASA CR-111849, June 1971, page 37.

3. Ibid, page 12.

4. Perry, R. H., Chemical Engineer's Handbook, McGraw Hill, 4th Edition, 1962, page 3-159.

5. Treybal, R. E.; Mass Transfer Operations, McGraw Hill (1955), page 453-457.

VLH20

1.0 Purpose

This routine is used to calculate the equilibrium partial pressures of water vapor over IR-45 solid amine resin. This pressure is assumed to be independent of CO_2 loading in the bed.

2.0 Use

This function is used by subroutine COABS, SDESRP, VACDSP, and SSS0R (lower level subroutines for COSORP) to determine the equilibrium partial pressure for specified values of water loading and temperature. This pressure is then used to determine the mass transfer rate of water vapor from the bed to the carrier gas flowing through the bed.

3.0 Calling Sequence

Z = VLH20 (W,T)

Function Value or Argument	Type	I/O	Description
VLH20 ( )	R	0	Equilibrium partial pressure $(\frac{lb}{in^2})$
W	R	I	Water bed loading $(\frac{lb\ H_2O}{lb_{dry\ resin}})$
T	R	I	Temperature (F)

Example:

Z = VLH20 (RX(J+04), RX(J+06))

4.0 Output

Returns a value for VLH20 (   ) as described above.

5.0 Method

The equilibrium partial pressure of water vapor is calculated by equation (1) and (2) presented below. Equation (1) is based on a least square fit of data presented in Reference 1 for data at 77°F. The data is extended to other temperatures (T) by use of techniques described in Reference 2.

$$P^{*}_{H_2O,77} = .0996972 + .246341W + 68.7792W^2 - 700.607W^3 + 262548W^4 - 3409.82W^5 \qquad (1)$$

and

$$P^{*}_{H_2O,T} = P^{Sat}_{H_2O,T} \left[\frac{P^{*}_{H_2O,77}}{P^{Sat}_{H_2O,77}} \right]^{\frac{537}{T}} \qquad (2)$$

where:

$P^{*}_{H_2O,77}$ = equilibrium vapor pressure over IR-45 with water loading W and temperature T (psia)

$P^{Sat}_{H_2O,77}$ = saturation pressure for water at 77°F (psia)

$P^{Sat}_{H_2O,77}$ = saturation pressure for water at temperature T (psia)

$P^{*}_{H_2O,T}$ = equilibrium vapor pressures over IR-45 with water loading W, and temperature T (psia)

T = Bed temperature (°R)

W = Bed water loading $\frac{lb_{H_2O}}{lb_{dry\ resin}}$

6.0 References

1. Tepper, F.; Vancheri, F.; Samuel, W. and Vdavcak: Development of a Regenerable Carbon Dioxide Removal System NASA CR-66571 (MSA Research Corporation) Jan 1968, p41.

2. Treybal, R. E.; Mass Transfer Operations, McGraw-Hill (1955) p. 453-457.

APPENDIX C

MODIFIED SUBROUTINES

Reference Location	Description	Data Type
55	Thermal conductance between surface of insulation and ambient gas (Btu/hr-°F)	I(R)
56	Convective heat loss to ambient gas (Btu/hr)	0
57	Ambient radiation wall temperature (°F)	I(R)
58	Thermal radiation $\mathcal{F}$A factor from surface of insulation to ambient wall (ft^2)	I(R)
59	Radiative heat loss to ambient wall (Btu/hr)	0
60	Structure temperature for heat shorts (°F)	I(R)
61	Thermal conductance between module and structure temperature (Btu/hr-°F)	I(R)
62	Conductive heat loss to structure (Btu/hr)	0
63	Insulation surface temperature (°F)	0
64	Conductance between module and outer surface of insulation (Btu/hr-°F) (If R(64)=0, there is no insulation)	I(R)

2.4 Steady State K-Array Data

Reference Location	Description	Data Type
16	Component number of alternate component	I(R)
17	Table number for bi-variant curve for cell voltage = -N use constant value for cell voltage in R(75) = N table number 1st independent variable = current density (amps/ft^2) 2nd independent variable = temperature (°F)	I(0)
18	Table number for bi-variant curve for CO_2 transfer rate (lb/hr-amp-cell) = -N use constant value in R(66) = N table number 1st independent variable = current density (amps/ft^2) 2nd independent variable = temperature (°F)	I(0)

2.5 Steady State/Transient V-Array Data

Reference Location	Description	Data Type
65	Removal rate of CO_2 (lb/hr)	0
66	Transfer rate of CO_2 (lb/hr-amp-cell)	I(R)
67	Desired module temperature (°F)	I(R)
68	Heater turnoff temperature (°F)	I(R)
69	Heater turnon temperature (°F)	I(R)
70	Actual temperature of module (°F)	I(R),0

Reference Location	Description	Data Type
71	Design of current density (amp/ft^2)	I(R)
72	Area of a cell (ft^2)	I(R)
73	Number of cells in module	I(R)
74	Total current (amps)	0
75	Voltage per cell (volts)	I(R)
76	Electrical power (watts)	0
77	Relative humidity in exit cathode gases (%)	I(R)
78	Relative humidity in exit anode gases (%)	I(R)
79	Water loss from electrolyte, all cells (lb/hr)	0
80	External water makeup rate to matrix, all cells equally divided (lb/hr) [Applies if NSTR(1) = 1. Can be a fixed input or GPØLY calculated.]	I(R)
81	Weight of water per cell in matrix (lb)	I(R), 0
82	Weight of $C_{s_2} CO_3$ per cell in matrix (lb)	I(R),0
83	Desired solids concentration in matrix (%)	I(R)
84	Actual solids concentration in matrix (%)	I(R), 0
85	Vapor pressure of water over electrolyte (psia)	0
86	Total pressure of stage (psia)	I(R)
87	Thermal capacitance of stage (Btu/°F) (not required for steady state)	I(R)
88	Coolant flow to stage (lb/hr)	0
89	Coolant c_p to stage (Btu/lb-°F)	0
90	Coolant inlet temperature (°F)	0
91	Coolant outlet temperature (°F)	0
92	Heat transfer conductance from coolant to cell (Btu/hr-°F)-cell)	I(R)
93	Heat transfer to coolant (Btu/hr)	0
94	Additional heat source or sink to module (Btu/hr)	I(R)

3.0 Analytical Model Description

Mass Transfer Equations

CO_2: The transport of CO_2 from the cathode to the anode compartment is according to the equation.

$$\hat{W}_{CO_2} = r_{CO_2} * A_{cell} * j * N \qquad (1)$$

Reference Location	Description	Data Type
54	Ambient gas temperature (°R)	I(R)
55	Thermal conductance between surface of insulation and ambient gas (Btu/hr-°F)	I(R)
56	Convective heat loss to ambient gas (Btu/hr)	0
57	Ambient radiation wall temperature (°F)	I(R)
58	Thermal radiation $\mathcal{F}$A factor from surface of insulation to ambient wall (ft^2)	I(R)
59	Radiative heat loss to ambient wall (Btu/hr)	0
60	Structure temperature for heat shorts (°F)	I(R)
61	Thermal conductance between module and structure temperature (Btu/hr-°F)	I(R)
62	Conductive heat loss to structure (Btu/hr)	0
63	Insulation Surface Temperature (°F)	0
64	Conductance bwtween module and outer surface of insulation (Btu/hr-°F) (If R(64) = 0, there is no insulation)	I(R)

2.4 Steady State K-Array Data

Reference Location	Description	Data Type
16	Component number of alternate component	I(R)
17	Table number for bi-variant curve for cell voltage = -N use constant value for cell voltage in R(75) = N table number 1st independent variable = current density (amps/ft^2) 2nd independent variable = temperature (°F)	I(0)

2.5 Steady State/Transient V-Array Data

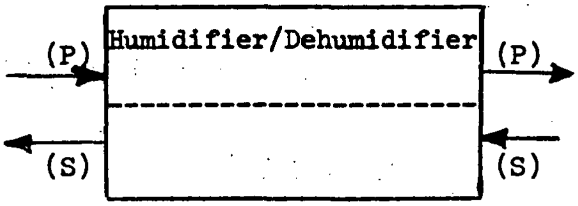
Reference Location	Description	Data Type
65	Removal efficiency of oxygen, $0 \le \eta \le 1$	I(R)
66	Not used	

Reference Location	Description	Data Type
67	Desired module temperature (°F)	I(R)
68	Heater turnoff temperature (°F)	I(R)
69	Heater turnon temperature (°F)	I(R)
70	Actual temperature of module (°F)	I(R),0
71	Design current density (amp/ft^2)	I(R)
72	Area of a cell (ft^2)	I(R)
73	Number of cells in module	I(R)
74	Total current (amps)	0
75	Voltage per cell (volts)	I(R)
76	Electrical power (watts)	0
77	Relative humidity in exit cathode gases (%)	I(R)
78	Relative humidity in exit anode gases (%)	I(R)
79	Water loss from electrolyte, all cells (lb/hr)	0
80	External water makeup rate to matrix, all cells equally divided (lb/hr) [Applies if NSTR(1) = 1; can be a fixed input or GP0LY calculated.]	I(R)
81	Weight of water per cell in matrix (lb)	I(R), 0
82	Weight of H_3PO_4 per cell in matrix (lb)	I(R), 0
83	Desired H_3 PO_4 concentration in matrix (%)	I(R)
84	Actual H_3PO_4 concentration in matrix (%)	I(R), 0
85	Vapor pressure of water over electrolyte (psia)	0
86	Total pressure of stage (psia)	I(R)
87	Thermal capacitance of stage (Btu/°F) (not required for steady state)	I(R)
88	Coolant flow to stage (lb/hr)	0
89	Coolant c_p to stage (Btu/lb-°F)	0
90	Coolant inlet temperature (°F)	0
91	Coolant outlet temperature (°F)	0
92	Heat transfer conductance from coolant to cell (Btu/hr-°F-cell)	I(R)
93	Heat transfer to coolant (Btu/hr)	0
94	Additional heat source or sink to module (Btu/hr) [Can be an external heater for thermal control]	I(R)

Component Subroutine No. 26 - Humidifier/Dehumidifier

1.0 Subroutine Description

This subroutine simulates a water vapor mass exchanger in terms of an over-all effectiveness factor similar to heat exchanger calculations. A schematic of the component is shown below.



Flow Codes 1, 2, or 3

FIGURE 1. HUMIDIFIER/DEHUMIDIFIER COMPONENT SCHEMATIC

2.0 Subroutine Data

2.1 General Notes

The flow streams may employ flow codes 1, 2, or 3.

2.2 Steady State V-Array Data

Reference Location	Description	Data Type
65	Effectiveness factor for mass transfer $0 \leq \eta \leq 1$	I(R)
66	Water transferred in exchanger (lb/hr)	0
67	Total pressure within exchanger (psia)	I(O)
68	Effectiveness factor for heat transfer $0 \leq \varepsilon \leq 1$	I(R)

3.0 Analytical Model Description

3.1 Vapor Transfer

The program computes the outlet partial pressure of stream j according to

$$p_{j,out} = p_{j,in} + n\,(p_{i,in} - p_{j,in}) \qquad (1)$$

where stream j is that stream which experiences the largest change in partial pressure of water. The + or - sign is chosen to give the correct direction of mass transfer, p_j is the partial pressure of water vapor in stream j, p_i is the partial pressure of water vapor in stream i, and n is the exchanger effectiveness. The subscripts in and out refer to conditions at the inlet and outlet of a stream, respectively.

Once the outlet partial pressure of the more "sensitive" stream is known, the water vapor transfer is easily calculated from the ideal gas laws.

The above definition of effectiveness parallels the definition used by Eckert and Drake "Heat and Mass Transfer" page 481 for heat transfer.

3.2 Thermal Transfer

The program computes the outlet temperature of the gas streams,primary and secondary, using the heat transfer effectiveness factor, ε, as follows:

$$T_{A,O} = T_{A,i} + \varepsilon \frac{C_{min}}{C_A} \; T_{B,i} - T_{A,i} \qquad (2)$$

$$T_{B,O} = T_{B,i} - \varepsilon \frac{C_{min}}{C_B} \; T_{B,i} - T_{A,i} \qquad (3)$$

where

$T_{A,i}$, $T_{A,O}$ - Inlet and Outlet temperature primary side.

$T_{B,i}$, $T_{B,O}$ - Inlet and Outlet temperature secondary side.

C_A, C_B - The hourly heat capacitance of primary and secondary side.

C_{min} - The smaller of C_A and C_B magnitudes.

ε - Heat transfer effectiveness factor, input value

The program does not compute external heat losses from the unit.

The above equations for temperature computations using the heat transfer effectiveness factor were obtained from Kreith "Principles of Heat Transfer" page 453.

REVISED 7-14-72

APPENDIX D

LISTING OF INPUT DATA
FOR SAMPLE PROBLEMS

```
*INSERT,GPOLY1,24
C       **************STEAM DESORBED AMINES**********************************
        IF( STEADY) RETURN
        IF( NPASS.NE.20) RETURN
        IF( N.NE.4) RETURN
C       SIMULATE SWITCHING FROM ABSORBING TO DESORBING MODE
C                    SWITCH SOLUTION PATHS
        M=1600000
        CALL SK(M,5,8)
        M=700000
        CALL SK(M,16,8)
        M= 600000
        CALL SK(M,15,8)
        M=1100000
        CALL SK(M,6,8)
C                    SWITCH FLOW SOURCES
        M=1602
        CALL SK(M,7,2)
        M=602
        CALL SK(M,11,2)
        M=1502
        CALL SK(M,6,2)
        M=502
        CALL SK(M,16,2)
C                    SWITCH MODES
        M=1
        CALL SK(M,6,22)
        M=0
        CALL SK(M,16,22)
C                    SWITCH PROFILES
        M=1
        CALL SK(M,6,23)
        M=1
        CALL SK(M,16,23)
 TAPE
 BASIC                        20        13        16     YEA        NAY
 CASE          STEAM DESORBED RESIN CONCEPT
  $CASE1
        KCHOUT=0, KPRNT=006, KPTINV(1)=001, KRUN=1,
        TMIN=-460., TMAX=2000., WTMAX=10000., MAXSLP=20,
        DTIME=060., START=0., TIMEMX=2400., MAXSSI= 2,
        MINSSI=1 $
  $PROP1
        CPCO2=.197, CPDIL=.22, VISGAS=.045, WTMTC=16.,
        XKGAS=.0147,WTMDIL=28.,WTMCON=18., CPCONV=.44,
        CPCONL=1., CP(1)=1.0,  RHO(1)=62.4,VISC(1)=2.37,
        WTM(1)=18.,XK(1)=0.347,
        CP(2)=.451,  RHO(2)=.0372,   VISC(2)=3.13E-2,
        WTM(2)=18.,  XK(2)=.0145,CPOXY=.22     $
 ID**    3      FLOW MIX
 KBAS    3       7          9                   -20                 10
 ID**    4      SUBSYSTEM BLOWER
 NSTR    4     0030
 KBAS    4      23         14 2                                      5
 VARY    4   91 60.            HEAT ADDED TO GAS STREAM(WATTS)
 ID**    5      BY PASS VALVE
 NSTR    5     0
 KBAS    5      10         4 2                 2                     6
 VARY   05   65 .0001          FRACTION OF FLOWBYPASSING CONCENTRATOR
 ID**    6      ABSORBING SOLID AMINES BED
```

```
NSTR    6    2010023          15   00
KBAS    6     36108            5 2                                            7
KARY    6   16               0       BED ABSORBING(DURING STEADY STATE)
KARY    6   17              -1       USE BUILT-IN RELATIONSHIP FOR H2O ISOTHERMS
KARY    6   18               1       INTERPOLATE TABLE FOR CO2 EQUIL PART PRESS.
KARY    6   21              12       NUMBER OF BED ELEMENTS
KARY    6   22               0       BED ABSORBING(DURING TRANSIENT)
VARY    6   65 ,018
VARY    6   66 ,22
VARY    6   68 28,8                  BULK DENSITY(LB/HR)
VARY    6   69 ,00115                PELLET DIAMETER(FT)
VARY    6   70 ,40                   VOID FRACTION
VARY    6   71 3130,                 SUPERFICIAL SURFACE AREA(SQ FT/OU FT)
VARY    6   72 1,                    SPHERICITY
VARY    6   73 1,                    CHANNELING FACTOR
VARY    6   75 1,57                  BED FRONTAL AREA(SQ FT)
VARY    6   76 ,458                  BED LENGTH(FT)
VARY    6   77 3,23
VARY    6   78 3,63
VARY    6   79 250,                  HEAT OF SORPTION-CO2-(BTU/LB)
VARY    6   80 ,536                  BINARY DIFFUSION COEF,-CO2/AIR-(SQ FT/HR)
VARY   06   81 14,       E-4         OVERALL MASS TRANS, COEF, FOR CO2(DESORPTION)
VARY    6   82 6,8      E-04         OVERALL MASS TRANS, COEF, FOR CO2(ABSORPTION)
VARY    6   83 1400,                 HEAT OF SORPTION-H2O-(BTU/LB)
VARY    6   84 ,854                  BINARY DIFFUSION COEF,-H2O/AIR-(SQ FT/HR)
VARY   06   85 22,       E-4         OVERALL MASS TRANS, COEF, FOR H2O(DESORPTION)
VARY    6   86 6,8       E-4         OVERALL MASS TRANS, COEF, FOR H2O(ABSORPTION)
VARY    6   98 75,
VARY    6 100 ,26                    DRY RESIN HEAT CAPACITY(BUT/LB-F)
VARY    6 103 ,5                     MULTIPLYING FACTOR FOR COMPUTING INTERVAL
VARY    6 104 0,
VARY    6 108 200,                   INITIAL VALUE GAS OUTLET TEMPERATURE(F)
VARY    6 109 200,                   INITIAL VALUE BED TEMPERATURE(F)
VARY    6 112 760,                   INITIAL VALUE AIR PARTIAL PRESSURE(MMHG)
VARY   06 107 ,26847                 INITIAL H2O LOADING               (LB/LB)
VARY   06 116 ,26912
VARY   06 125 ,26975
VARY   06 134 ,27036
VARY   06 143 ,27079
VARY   06 152 ,27116
VARY   06 161 ,27154
VARY   06 170 ,27194
VARY   06 179 ,27239
VARY   06 188 ,27291
VARY   06 197 ,27356
VARY   06 206 ,2741
VARY    6 105 ,02383                 INITIAL CO2 BED LOADING           (LB/LB)
VARY    6 114 ,02225
VARY    6 123 ,020738
VARY    6 132 ,019277
VARY    6 141 ,01826
VARY    6 150 ,017396
VARY    6 159 ,016539
VARY    6 168 ,0156176
VARY    6 177 ,014555
VARY    6 186 ,01323
VARY    6 195 ,01136
VARY    6 204 ,0083
ID--    7     AIR CONDENSING HEAT EXCHANGER
NSTR    7    2110001              1
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KBAS    7      4            6 2                  -17 0   1           5
VARY    7  66 50.            ESTIMATED VALUE COND. UA
~~VARY    7  74 3.             MAXIMUM NTU~~
VARY    7  75 55.            DESIRED TEMP. FOR AIR TO CABIN(F)
VARY    7  85 10.            TIME CONSTANT(SECONDS)
~~ID**    8      AIR CHARCOAL FILTER~~
NSTR    8      3
KBAS    8      11           7 2                                      9
~~VARY    8  77 .01            TRACE CONTAMINATES REMOVAL EFFICIENCY~~
ID**    9      MAKEUP WATER TANK
NSTR    9      1210
~~KBAS    9      30             0  1                                  20~~
VARY    9  01 4.0            TOTAL FLOW WATER FROM ACCUMULATOR(LB/HR)
VARY    9  02 75.            TEMP. OF WATER FROM ACCUMULATOR(F)
~~VARY    9  04 14.7           PRESS.OF WATER FROM ACCUMULATOR(LB SQ IN)~~
VARY    9  54 75.            AMBIENT GAS TEMPERATURE(F)
VARY    9  55 1.             UA TO SURROUNDINGS(BTU/HR-F)
~~VARY    9  57 75.            AMBIENT RADIATION TEMPERATURE(F)~~
VARY    9  60 75.            AMBIENT STRUCTURAL TEMPERATURE-F)
VARY    9  67 31.2           TOTAL MASS IN TANK     (LB)
~~VARY    9  68 75.            FLUID TEMPERATURE(F)~~
VARY    9  69 0.5            FLUID VOLUME(CU FT)
VARY    9  70 14.7           FLUID PRESSURE(PSIA)
~~VARY    9  73 31.2           MASS OF H2O IN TANK     (LB)~~
VARY    9  90 0.             THERMAL CAPACITANCE(BUT/F)
VARY    9  91 0.             THERMAL CONDUCTANCE FLUID/TANK WALL(BUT/HR-F)
~~VARY    9  92 5.             MAXIMUM ALLOWABLE TEMP.CHANGE(F)~~
ID**   10      WATER ACCUMULATOR
NSTR   10      1210
~~KBAS   10      30           3 0  1                                  19~~
VARY   10  01 4.0            TOTAL FLOW FROM WATER MAKEUP TANK(LB/HR)
VARY   10  02 75.            TEMP.OF WATER FROM MAKEUP TANK(F)
~~VARY   10  04 14.7           PRESS.OF WATER FROM MAKEUP TANK(LB/SQ IN)~~
VARY   10  54 75.            AMBIENT GAS TEMPERATURE(F)
VARY   10  55 1.             UA TO SURROUNDINGS(BTU/HR-F)
~~VARY   10  57 75.            AMBIENT RADIATION TEMPERATURE(F)~~
VARY   10  60 75.            AMBIENT STRUCTURAL TEMPERATURE(F)
VARY   10  67 4.7            TOTAL MASS IN TANK     (LB)
~~VARY   10  68 75.            FLUID TEMPERATURE(F)~~
VARY   10  69 .075           FLUID VOLUME(CU FT)
VARY   10  70 14.7           FLUID PRESSURE(PSIA)
~~VARY   10  73 4.7            MASS OF H2O IN TANK     (LB)~~
VARY   10  90                THERMAL CAPACITANCE(BTU/F)
VARY   10  91                THERMAL CONDUCTANCE FLUID/TANK WALL(BTU/HR-F)
~~VARY   10  92 5.             MAXIMUM ALLOWABLE TEMP.CHANGE(F)~~
ID**   11      DESORBED CO2 FLOW COMPRESSOR
NSTR   11      003
~~KBAS   11      23          16 2                                     12~~
VARY   11  91  10.           HEAT ADDED TO GAS STREAM(WATTS)
ID**   12      STEAM CONDENSING HEAT EXCHANGER
~~NSTR   12      2110001~~
KBAS   12      4           11 2                  -18 0   1           13
VARY   12  66 50.            ESTIMATED VALUE COND. UA
~~VARY   12  74 3.             MAXIMUM NTU~~
VARY   12  75 55.            DESIRED TEMP. FOR AIR(F)
VARY   12  85 10.            TIME CONSTANT(SECONDS)
~~ID**   13      CO2 ACCUMULATOR~~
NSTR   13      0210
KBAS   13      30          12 2                                       4
~~VARY   13  01 .575           CO2 USE RATE                      (LB/HR)~~
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 VARY  13  54 75,             AMBIENT TEMPERATURE                  (F)
 VARY  13  55 2,              UA INSULATION/SURROUNDINGS           (BTU/HR-F)
~~VARY  13  67 ,307            TOTAL MASS  IN TANK  (LB)~~
 VARY  13  69 2,0             TANK VOLUME                          (CU FT)
 VARY  13  70 20,             ACCUMULATOR PRESSURE  (PSIA
~~VARY  13  78 ,307            MASS  OF  CO2 IN TANK (LB~~
 ID**  14     SOURCE OF FLOW TO SYSTEM(DUMMY COMPONENT)
 NSTR  14
~~KBAS  14     49              2~~
 VARY  14   1 84,867          TOTAL FLOW TO SUBSYSTEM(LB/HR)
 VARY  14   2 75,               TEMPERATURE(F)
~~VARY  14   4 14,7              PRESSURE(PSIA)~~
 VARY  14   6 ,76               WATER VAPOR(LB/HR)
 VARY  14  10 19,4              OXYGEN(LB/HR)
~~VARY  14  11 64,2              NITROGEN(LB/HR)~~
 VARY  14  12 ,507              CARBON DIOXIDE(LB/HR)
 VARY  14  13 ,02             TRACE CONTAMINATES                   (LB/HR)
~~ID**  15     STEAM BOILER(GENERATOR)~~
 KBAS  15     27          19 2                                              16
 VARY  15  66 20,             DEGREES SUPERHEAT                    (F)
~~NSTR  15     01~~
 ID**  16     DESORBING SOLID AMINES BED
 NSTR  16    201002300     15   0
~~KBAS  16     36108        15 2                                             11~~
 KARY  16  16            1    BED DESORBING DURING STEADY STATE
 KARY  16  17           -1    USE BUILT IN ISOTHERM DATA FOR H2O
~~KARY  16  18            1    INTERPOLATE TABLE FOR CO2 EQUIL PART PRESS.~~
 KARY  16  21           19    NUMBER OF BED ELEMENTS
 KARY  16  22            1    BED DESORBING DURING TRANSIENT
~~VARY  16  65 ,0075           AVERAGE CO2 BED LOADING(LB/LB)~~
 VARY  16  66 ,22             AVERAGE H2O BED LOADING
 VARY  16  68 28,8            BULK DENSITY(LB/CU FT)
~~VARY  16  69 ,00115          PELLET DIAMETER(FT)~~
 VARY  16  70 ,40             VOID FRACTION
 VARY  16  71 3130,           SUPERFICIAL SURFACE AREA(SQ FT/ CU FT)
~~VARY  16  72 1,              SPHERICITY~~
 VARY  16  73 1,              CHANNELING FACTOR
 VARY  16  75 1,57            BED FRONTAL AREA(SQ FT)
~~VARY  16  76 ,458            BED LENGTH(FT)~~
 VARY  16  77 3,23
 VARY  16  78 3,22
~~VARY  16  79 250,            HEAT OF SORPTION-CO2-(BTU/LB)~~
 VARY  16  80 ,536            BINARY DIFFUSION COEF,-CO2/AIR-(SQ FT/HR)
 VARY  16  81 14,      E-4    OVERALL MASS TRANS, COEF, FOR CO2(DESORPTION)
~~VARY  16  82 6,8     E-04    OVERALL MASS TRANS, COEF, FOR CO2(ABSORPTION)~~
 VARY  16  83 1400,           HEAT OF SORPTION-H2O-(BTU/LB)
 VARY  16  84 ,854            BINARY DIFFUSION COEF,-H2O/AIR-(SQ FT/HR)
~~VARY  16  85 22,      E-4    OVERALL MASS TRANS, COEF, FOR H2O(DESORPTION)~~
 VARY  16  86 6,8      E-6    OVERALL MASS TRANS, COEF, FOR H2O(ABSORPTION)
 VARY  16  99 0,50            DURATION DESORPTION CYCLE       (HOURS)
5~~VARY  16 100 ,26            DRY RESIN SPECIFIC HEAT(BUT/LB-F)~~
 VARY  16 103 ,5              MULTIPLYING FACTOR FOR COMPUTING INTERVAL
 VARY  16 104 0,
4~~VARY  16 108 75,            INITIAL GAS OUTLET TEMPERATURE(F)~~
 VARY  16 109 75,             INITIAL BED TEMPERATURE(F)
 VARY  16 112 760,            INITIAL VALUE AIR PARTIAL PRESSURE(MM HG)
3~~VARY  16 107 ,18070         INITIAL H2O LOADING              (LB/LB)~~
 VARY  16 116 ,18068
 VARY  16 125 ,18068
2~~VARY  16 134 ,18068~~
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VARY  16 143 .18067
VARY  16 152 .18059
VARY  16 161 .18029
VARY  16 170 .17938
VARY  16 179 .17692
VARY  16 188 .17304
VARY  16 197 .16597
VARY  16 206 .16245
VARY  16 105 .0155              INITIAL CO2 LOADING                (LB/LB)
VARY  16 114 .0155
VARY  16 123 .0156
VARY  16 132 .0156
VARY  16 141 .0156
VARY  16 150 .0156
VARY  16 159 .0157
VARY  16 168 .01659
VARY  16 177 .0325
VARY  16 186 .0485
VARY  16 195 .0496
VARY  16 204 .0481
ID**  17      SOURCE OF COOLANT(DUMMY COMPONENT)
NSTR  17
KBAS  17      49                0   1
VARY  17    1  200.             TOTAL COOLANT FLOW TO PROCESS AIR CONDENSER(LB/HR)
VARY  17    2 40.                 TEMPERATURE(F)
VARY  17    4 14.7                PRESSURE(PSIA)
ID**  18      SOURCE OF COOLANT(DUMMY COMPONENT)
NSTR  18
KBAS  18      49                0   1
VARY  18    1  200.             TOTAL COOLANT FLOW TO DESORBED GAS CONDENSER(LB/HR)
VARY  18    2 40.                 TEMPERATURE(F)
VARY  18    4 14.7                PRESSURE(PSIA)
ID**  19      WATER METERING PUMP
NSTR  19     0002
KBAS  19      22             10 0   1                                       15
VARY  19   85 15.               HEAT INPUT TO FLUID BY PUMP(WATTS)
KBAS  20      12                0                                           3
VARY  20   03 14.7              CONDENSATE TEMPERATURE
KARY  20   16              9
KARY  20   17              7
KARY  20   18             12
TABL   1  1    3                8     5    LOG   LIN   LIN
TITL   1  2 IR-45 EQUILIBRIUM ISOTHERMS(24.5 WT PER CENT H20) PPC02 VS LOADING
VALU   1 11 3I              74.         100.        130.        180.        250.
VALU   1 12 3D 0.           0.0001      0.0001      0.0001      0.0001      .0001
VALU   1 13 3D .005         .11         .16         .30         .50         .78
VALU   1 14 3D .01          .13         .26         .87         2.0         3.58
VALU   1 15 3D .02          .2          .69         4.0         20.         42.4
VALU   1 16 3D .03          .47         1.85        11.         85.         189.
VALU   1 17 3D .035         .77         3.0         16.5        135.        303.
VALU   1 18 3D .040         1.4         5.0         25.         220.        492.
VALU   1 19 3D .045         2.5         8.          37.         345.        653.
PLOT        6  98  0.           230.        ABSORBING BED AVER. BED TEMP.(F)
PLOT        6  65  0.           .05         ABSORBING BED AVG. CO2 LOADING(LB/LB)
PLOT        6  66  0.           .30         ABSORBING BED AVG. H2O LOADING(LB/LB)
PLOT        6  12  0.           10.         ABSORBING BED CO2 FLOW OUT(LB/HR)
PLOT        6   6  0.           20.         ABSORBING BED H2O FLOW OUT(LB/HR)
PLOT        6 207  0.           230.        ABSORBING BED GAS TEMP OUT(F)
PLOT        6 203  0.           760.        ABSORBING BED CO2 PARTIAL PRESSURE OUT(MM)
PLOT        6 205  0.           760.        ABSORBING BED H2O PARTIAL PRESSURE OUT(MM)
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PLOT        16   98   0.           230.        DESORBING BED AVER. BED TEMP.(F)
PLOT        16   65   0.           .05         DESORBING BED AVG. CO2 LOADING(LB/LB)
PLOT        16   66   0.           .30         DESORBING BED AVG. H2O LOADING(LB/LB)
[illegible]OT        16   12   0.           10.         DESORBING BED CO2 FLOW OUT(LB/HR)
PLOT        16    6   0.           20.         DESORBING BED H2O FLOW OUT(LB/HR)
PLOT        16  207   0.           230.        DESORBING BED GAS TEMP OUT(F)
PLOT        16  203   0.           760.        DESORBING BED CO2 PARTIAL PRESSURE OUT(MM)
PLOT        16  205   0.           760.        DESORBING BED H2O PARTIAL PRESSURE OUT(MM)
ENDC
ENDR
*
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*INSERT,GPOLY1,24
C       ***************VACUUM DESORBED AMINES**********************************
        IF( STEADY) GO TO 10
        IF¬ NPASS,GT,1< KCHOUT=0
        IF( N,NE,12) RETURN
        R(01)= 0,6
        V0801=VV(09,01)
        V0805= VV(09,05)
        V0806= VV(09,06)
        V0810= VV(09,10)
        V0811= VV(09,11)
        V0812= VV(09,12)
        V0813= VV(09,13)
        CALL SV(V0801,08;01)
        CALL SV(V0805,08;05)
        CALL SV(V0806,08;06)
        CALL SV(V0810,08;10)
        CALL SV(V0811,08;11)
        CALL SV(V0812,08;12)
        CALL SV(V0813,08;13)
     10 CONTINUE
        IF( N,NE,12) RETURN
        R(01)= A(01)
TAPE
BASIC            1        12       12               YEA        NAY
CASE        THERMAL/VACUUM DESORBED SOLID AMINES
 $CASE1
        KCHOUT=0, KPRNT=006, KPTINV(1)=030, KRUN=1,
        TMIN==460,, TMAX=2000,, WTMAX=10000,,MAXSLP=30,
        DTIME=2,,  START=0,, TIMEMX=1200,, MAXSSI=2,
        MINSSI=1 $
 $PROP1
        CPCO2=,197, CPDIL=,22, VISGAS=,045, WTMTC=16,,
        XKGAS=,0147,WTMDIL=28,,WTMCON=18,,CPCONV=,44,
        CPCONL=1,, CP(1)=1,, RHO(1)=62,4, VISC(1)=2,37,
        WTM(1)=18,, XK(1)=,347,
        CP(2)=1, , RHO(2)=60,1,  VISC(2)=,738,
        CPOXY=,22,CPTC=,50,
        WTM(2)=18,, XK(2)=,394   $
ID**     1      SOURCE OF CABIN AIR FLOW TO SUBSYSTEM
KBAS     1      49                  2
NSTR    01
VARY    01    1 84,87           TOTAL FLOW TO SUBSYSTEM            (LB/HR)
VARY    01    2 75,
VARY    01    4 14,7
VARY    01    6 0,766
VARY    01   10 19,4
VARY    01   11 64,23
VARY    01   12 ,628
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VARY  01  13 ,01
ID**   2      SUBSYSTEM BLOWER
~~KBAS   2      23               1 2                                               3~~
 TR   02    003
VARY  02  91 60,             HEAT ADDED TO GAS STREAM
~~ID**   3      AIR BYPASS VALVE~~
KBAS   3      10               2 2                                               6
NSTR  03
~~VARY  03  65 ,001           FRACTION OF TOTAL FLOW BYBASSIN SUBSYSTEM~~
ID**   5      SOURCE OF COOLANT FOR ABSORRING BED(COOL WATER)
ID**   4      SOURCE OF HOT FLUID FOR DESIRBING BED(HOT WATER)
~~KBAS   4      49                0   2~~
NSTR  04
VARY   4   1 270,             FLOWRATE                              (LB/HR)
~~VARY   4   2 200,             TEMPERATURE                           (F)~~
VARY   4   4 14,7             PRESSURE                              (PSIA)
KBAS   5      49                0   1
~~NSTR  05~~
VARY   5   1 270,             FLOWRATE                              (LB/HR)
VARY   5   2 55,              TEMPERATURE                           (F)
~~VARY   5   4 14,7             PRESSURE                              (PSIA)~~
ID**   6      ABSORBING SOLID AMINES BED
KBAS   6      36108          3 2                      -5 0   1                   7
~~NSTR   6     2131          11~~
KARY   6  16             0    BED ABSORBING(STEADY STATE)
KARY   6  17            -1    USE BUILT-IN H2O ISOTHERMS
~~KARY   6  18             0    INTERPOLATE TABLE FOR CO2 PART,PRESS~~
KARY   6  21            19    NUMBER OF BED ELEMENTS
 ARY   6  22             0    BED ABSORBING(TRANSIENT)
~~ ARY   6  57 ,5~~
VARY   6  55 ,5
VARY   6  65 ,018
~~VARY   6  66 ,22~~
VARY   6  68 28,8             BULK DENSITY(LB/HR)
VARY   6  69 ,00115           PELLET DIAMETER(FT)
~~VARY   6  70 ,40             VOID FRACTION~~
VARY   6  71 3130,            SUPERFICIAL SURFACE AREA(SQ FT/CU FT)
VARY   6  72 1,               SPHERICITY
~~VARY   6  73 1,               CHANNELING FACTOR~~
VARY   6  75 1,57             BED FRONTAL AREA(SQ FT)
VARY   6  76 ,458             BED LENGTH(FT)
~~VARY   6  77 3,23~~
VARY   6  78 3,63
VARY   6  79 250,             HEAT OF SORPTION-CO2-(BTU/LB)
~~VARY   6  80 ,536             BINARY DIFFUSION COEF,-CO2/AIR-(SQ FT/HR)~~
VARY   6  82 6,8    E-04      OVERALL MASS TRANS, COEF, FOR CO2(ABSORPTION)
VARY   6  83 1400,            HEAT OF SORPTION-H2O-(BTU/LB)
~~VARY   6  84 ,854             BINARY DIFFUSION COEF,-H2O/AIR-(SQ FT/HR)~~
VARY   6  86 6,8     E-4      OVERALL MASS TRANS, COEF, FOR H2O(ABSORPTION)
VARY   6  87 0,               U  CORE/GAS                           (BTU/HR-SQ FT-F)
5 ~~VARY   6  88 1,               A  CORE/GAS                           (SQ FT)~~
VARY   6  89 146,             U  CORE/BED                           (BTU/HR-SQ FT-F)
VARY   6  90 1,               A  CORE/BED                           (SQ FT)
4 ~~VARY   6  91 1,               A  GAS/CANNISTER                      (SQ FT)~~
 ARY   6  92 0,05             U  GAS/CANNISTER                      (BTU/HR-SQ FT-F)
VARY   6  93 146,             U  FLUID/CORE                         (BTU/HR-SQ FT-F)
3 ~~VARY   6  94 1,               A  FLUID/CORE                         (SQ FT)~~
VARY   6  98 75,
VARY   6 100 ,26              DRY RESIN HEAT CAPACITY(BTU/LB-F)
2 ~~VARY   6 102 1,0~~
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VARY    6 101 ,208
VARY    6 103 ,5                  MULTIPLYING FACTOR FOR COMPUTING INTERVAL
~~VARY    6 104 ,9~~
 RY    6 105 ,018                INITIAL VALUE CO2 LOADING(LB SORBATE/LB DRY RESIN)
VARY    6 106
~~VARY    6 107 ,25                 INITIAL VALUE H20 LOADING(LB SORBATE/LB DRY RESIN)~~
VARY    6 108 200,                INITIAL VALUE GAS OUTLET TEMPERATURE(F)
VARY    6 109 200,                INITIAL VALUE BED TEMPERATURE(F)
~~VARY    6 112 760,                INITIAL VALUE AIR PARTIAL PRESSURE(MM HG)~~
ID**    7      CHARCOAL TRAP
KBAS    7      11           6 2                                          9
~~NSTR   07     3~~
VARY   07   77 ,01                (1=TRACE CONTAMINATES REMOVAL EFFICIENCY)
ID**    8      DESORBING SOLID AMINES BED
~~KBAS    8      34108              2                   =4 0  2           9~~
NSTR    8     2131          11    00
KARY    8   16              1     BED DESORBING(DURING STEADY STATE)
KARY    8   17             =1     USE BUILD=IN RELATIONS HIP FOR H20 ISOTHERMS
KARY    8   18              2     INTERPOLATE TABLE FOR CO2 PART,PRESS
KARY    8   21             12     NUMBER OF BED ELEMENTS
~~KARY    8   22              1     BED DESORBING(DURING TRANSIENT)~~
VARY    8   65 ,018               SS AVERAGE CO2 BED LOADING      (LB CO2/LB BED)
VARY    8   66 ,22                SS AVERAGE H20 BED LOADING      (LB H20/LB BED)
~~VARY    8   68 28,8               BULD DENSITY                    (LB/CU FT)~~
VARY    8   69 ,00115             PELLET DIAMETER                 (FT)
VARY    8   70 ,40                VOID FRACTION
~~VARY    8   71 3130,              SUPERFICIAL SURFACE AREA        (SQ FT/CU FT)~~
VARY    8   72 1,                 SPHERICITY
 ARY    8   73 1,                 CHANNELING FACTOR
~~ ARY    8   75 1,57               BED FRONTAL AREA                (SQ FT)~~
VARY    8   76 ,458               BED LENGTH                      (FT)
VARY    8   77 3,23               UA GAS/PELLETS DURING ABSORPTION(BTU/HR=S4 FT=F)
~~VARY    8   79 250,               HEAT OF ABSORPTION=CO2          (BTU/LB)~~
VARY    8   80 ,536               BINARY DIFFUSION COEF,=CO2/AIR  (SQ FT/HR)
VARY    8   82 6,8    E=04        OVERALL MASS TRANS, COEF,FOR CO2=ABSORPTION
~~VARY    8   83 1400,              HEAT OF SORPTION=H20=       (BTU/LB)~~
VARY    8   84 ,854               BINARY DIFFUSION COEF,=H20/AIR  (SQ FT/ HR)
VARY    8   86 6,8     E=6        OVERALL MASS TRANS, COEF, H20=ABSORPTION
~~VARY    8   87 0,                 U  CORE/GAS                     (BTU/HR=SQ FT=F)~~
VARY    8   88 1,                 A  CORE/GAS                     (SQ FT)
VARY    8   89 146,               U  CORE/BED                     (BTU/HR=SQ FT=F)
~~VARY    8   90 1,                 A  CORE/BED                     (SQ FT)~~
VARY    8   91 1,                 A  GAS/CANNISTER                (SQ FT)
VARY    8   92 0,                 U  GAS/CANNISTER                (BTU/HR=SQ FT=F)
~~VARY    8   93 146,               U  FLUID/CORE                   (BTU/HR=SQ FT=F)~~
VARY    8   94 1,                 A  FLUID/CORE                   (SQ FT)
VARY    8   98 180,
~~VARY    8   99 ,25                DURATION OF DESORPTION CYCLE    (HOURS)~~
VARY    8 100 ,26                 DRY RESIN HEAT CAPACITY         (BTU/LB=F)
VARY    8 101 ,208                HX THERMAL CAPACITANCE          (BTU/F)
5 ~~VARY    8 102 1,0                 FLUID THERMAL CAPACITANCE       (BTU/F)~~
VARY    8 103 ,50                 MULTIPLYING FACTOR FOR COMPUTING INTERVAL
VARY    8 104 0,                  INITIAL VALUE CO2 PART,PRESSURE (MM HG)
4 ~~VARY    8 105 0,031               INITIAL VALUE CO2 BED LOADING   (LB/LB)~~
 ARY    8 106 20,                 INITIAL VALUE H20 PART,PRESSURE (MM HG)
VARY    8 107 ,25                 INITIAL VALUE H20 LOADING       (LB/LB)
3 ~~VARY    8 108 75,                 INITIAL VALUE GAS TEMPERATURE   (F)~~
VARY    8 109 75,                 INITIAL VALUE BED TEMPERATURE   (F)
VARY    8 110 75,                 HEAT EXCHANGER CORE TEMPERATURE (F)
2 ~~VARY    8 111 75,                 HEATING FLUID TEMPERATURE       (F)~~
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VARY    8 112 740,           INITIAL VALUE AIR PART,PRESSURE (MM HG)
ID**    9      VACUUM PUMP
KBAS    9      28            8 2                                                 10
   TR   9     111
VARY    9  75 20,            DISCHARGE PRESSURE                  (PSIA)
KARY    9  16            1   TABLE FOR COMPRESSOR FLOW
VARY    9  66 0,60           MOTOR EFFICIENTY                    (DIM)
VARY    9  67 0,40           AERODYNAMIC EFFICIENCY              (DIM)
VARY    9  71 0,             FRACTION Q LOST TO AMBIENT          (DIM)
VARY   09  74 1,3            POLYTROPIC EXPONENT
ID**   10      CONDESING HEAT EXCHANGER
KBAS   10       4            9 2                    -11     1                    12
NSTR   10     2000001        1
VARY   10  75 75,            DESIGN TEMPERATURE                  (F)
VARY   10  66 7,5            UA FOR HX
ID**   11      SOURCE OF COOLANT TO CONDENSING HEAT EXCHANGER
KBAS   11      49            0   2
NSTR   11
VARY   11   1 10,            FLOWRATE                            (LB/HR)
VARY   11   2 40,            TEMPERATURE                         (F)
VARY   11   4 14,7           PRESSURE                            (PSIA)
ID**   12      CO2 ACCUMULATOR
KBAS   12      30          10 2                                                  2
NSTR   12     0020
VARY   12  01 ,575           CO2 USE RATE                        (LB/HR)
VARY   12  54 75,            AMBIENT TEMPERATURE                 (F)
VARY   12  55 2,             UA INSULATION/SURROUNDINGS          (BTU/HR-F)
VARY   12  69 0,307          TOTAL MASS IN TANK(INITIALY)        (LB)
 ARY   12  78 0,307          MASS CO2 IN TANK(INITIALLY)         (LB)
 ARY   12  70 20,            TANK PRESSURE                       (PSIA)
TABL    1  1   3           11       4     LOG    LOG    LIN
TITL    1  2 VACUUM PUMP FLOW CHARACTERISTICS(LARGE PUMP)
VALU    1 11 3I              7,         14,7        30,         50,
VALU    1 12 3D 1,           4,15       4,35        4,8         5,
VALU    1 13 3D 5,           4,12       4,25        4,8         5,
VALU    1 14 3D 10,          3,35       4,15        4,5         5,
VALU    1 15 3D 30,          2,30       3,20        4,0         4,3
VALU    1 16 3D 50,          1,5        2,5         3,3         3,9
VALU    1 17 3D 70,          1,15       2,05        2,80        3,3
VALU    1 18 3D 100,         ,5         1,35        2,25        2,8
VALU    1 19 3D 118,         0,0001     1,25        2,15        2,6
VALU    1 20 3D 228,         0,0001     0,0001      0,8         1,2
VALU    1 21 3D 370,         0,0001     0,0001      0,0001      ,4
VALU    1 22 3D 420,         0,0001     0,0001      0,0001      0,0001
TABL    2  1   3            8       5     LOG    LIN    LIN
TITL    2  2 IR-45 EQUILIBRIUM ISOTHERMS(24,5 WT PER CENT H2O) PPCO2 VS LOADING
VALU    2 11 3I              74,        100,        130,        180,        250,
VALU    2 12 3D 0,           0,0001     0,0001      0,0001      0,0001      ,0001
VALU    2 13 3D ,005         ,11        ,16         ,30         ,50         ,78
VALU    2 14 3D ,01          ,13        ,26         ,87         2,0         3,58
VALU    2 15 3D ,02          ,2         ,69         4,0         20,         42,4
VALU    2 16 3D ,03          ,47        1,85        11,         85,         189,
VALU    2 17 3D ,035         ,77        3,0         16,5        135,        303,
VALU    2 18 3D ,040         1,4        5,0         25,         220,        492,
 ALU    2 19 3D ,045         2,5        8,          37,         345,        653,
ENDC
ENDR
*
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*INSERT,GPOLY1,24
C      **************CARBONATION CELL**********************************
       IF(N .NE. 18) GO TO 10
       VV12=VV(4,12)
       VV431=VV(4,31)
       VV401=VV(4,1)
       VV420=VV(4,20)
       VV720=100.*VV431/VV420
       VV721=100.* VV12/VV401
       VV722=VV(4,12)+VV(4,10)
       CALL SV(VV720,7,20)
       CALL SV(VV721,7,21)
       CALL SV(VV722,7,22)
       V480=VV(4,80)
       V880=VV(8,80)
       R(1) =    V480+V880
   10 CONTINUE
TAPE
BASIC           1       40       18       12     YEA       NAY
CASE         CARBONATION CELL CO2 CONCENTRATOR SYSTEM CHECKOUT
 $CASE1
  KCHOUT=0, KPRNT=6, KPTINV(1)=15,MAXSLP=7, MINSSI=2, KRUN=1, DTIME=30.,
  TIMEMX=3600.,MAXSSI=5, TMAX=250., TMIN=-450., WTMAX=1.E4 $
 $PROP1
  CP(1)=.239,RHO(1)=.16  ,VISC(1)= .036 ,WTM(1)=28.0   ,XK(1)=.007    ,
  CP(2)=1.,RHO(2)=62.4   ,VISC(2)= 3.6  ,WTM(2)=18.0   ,XK(2)=.325    ,
  CP(3)=.175,RHO(3)=.25  ,VISC(3)= .036 ,WTM(3)=44.0   ,XK(3)=.007    ,
   CPCONL=1., CPCONV=0.44, CPCO2=0.2, CPDIL=0.25, CPOXY=0.22, CPTC=0.2,
   GAMGAS=1.4, VISGAS=0.44, WTMCON=18., WTMDIL=28., WTMTC=20.,
   CPCO2 = .178,       WTMCON=18. ,
   XKGAS=0.146 $
ID**    1    1 DUMMY COMPONENT PROVIDING THE INLET FLOW TO CO2 REMOVAL SYSTEM USIN
ID**    1    2 THE CARBONATION CELL CONCEPT.
KBAS    1      49                2
VARY    1    1   211.987         TOTAL FLOW                                 (LB/HR)
VARY    1    2    70.            TEMPERATURE                                (F)
VARY    1    3   14.7            PRESSURE                                   (PSI)
VARY    1    4   14.7            PRESSURE                                   (PSI)
VARY    1    5  209.697          NON-CONDENSABLE FLOW                       (LB/HR)
VARY    1    6    2.29           VAPOR FLOW                                 (LB/HR)
VARY    1    8     .24           NON-CONDENSABLE SPECIFIC HEAT              (BTU/LB-F)
VARY    1    9  28.97            NON-CONDENSABLE MOLECULAR WEIGHT           (MOLES/LB)
VARY    1   10    49.3           OXYGEN FLOW                                (LB/HR)
VARY    1   11   159.13          DILUENT (N2) FLOW                          (LB/HR)
VARY    1   12     1.267         CO2 FLOW                                   (LB/HR)
ID**    2      BLOWER PASSING THE STREAM FROM COMPONENT 2 TO 3 SLIGHT INCREASE TEM
KBAS    2      23              1 2                                         3
NSTR    2     0030                   SUBROUTINE FAN ADD HEAT SPECIFIED IN R(91)
VARY    2   91    150.           HEAT ADDED TO GAS STREAM AS IT FLOWS THROUGH THE FAN
ID**    3      WATER VAPOR MASS EXCHANGER HUMIDIFIER/DEHUMIDIFIER
KBAS    3      26              2 2                  -4 2                 4
VARY    3   65      .95          EFFECTIVENESS FACTOR FOR MASS TRANSFER
VARY    3   68      .94          EFFECTIVENESS FACTOR FOR HEAT TRANSFER
ID**    4      FIRST STAGE OF ELECTROCHEMICAL CARBONATION CELL CO2 CONCENTRATOR SY
KBAS    4      24              3 2                   2                    6
NSTR    4     01                     POUNDS OF H2O AND TEMP. OF STAGE TRANSIENT
KARY    4   16          34       COMPONENT NUMBER OF COOLANT SUPPLY
VARY    4    1   231.00          FLOW                                       LB/HR
VARY    4    2    140.           TEMP                                       F
VARY    4    3   14.7            PRESS                                      PS1
VARY    4    4   14.7            PRESS                                      PS1
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 VARY    4   6   13,61      VAPOR FLOW                                    LB/HR
 VARY    4   8     ,24      SPECIFIC HEAT                                 BTU/LB-F
~~VARY    4   9   28,923     MOLECULAR WEIGHT                              LB/MOLE~~
 VARY    4  10   49,3       O2 FLOW                                       LB/HR
 VARY    4  11  159,13      N2 FLOW                                       LB/HR
 VARY    4  12     ,84      CO2 FLOW                                      LB/HR
 VARY    4  54    70,       AMBIENT GAS TEMPERATURE                       -F)
 VARY    4  55    0,1       THERMAL CONDUCTANCE BETWEEN SURFACE AND GAS (B/HR-F)
~~VARY    4  57   60,        AMBIENT RADIATION WALL TEMP                   (F)~~
 VARY    4  58    2,        THERMAL RADIATION FA FACTOR                   (FT**2)
 VARY    4  60   60,        STRUCTURE TEMP FOR HEAT SHORTS                (F)
~~VARY    4  61    ,1        THERMAL CONDUCTANCE BETWEEN MODULE/STRUC, (BTU/HR-F)~~
 VARY    4  66    ,00121    TRANSFR RATE OF CO2                     (LB/HR-AMP-CELL)
 VARY    4  67   140,       DESIRED MODULE TEMPERATURE                    (F)
~~VARY    4  68   142,       HEATER TURNOFF TEMPERATURE                    (F)~~
 VARY    4  69   138,       HEATER TURNOFF TEMPERATURE                    (F)
 VARY    4  70   140,       ACTUAL TEMPERATURE OF MODULE                  (F)
~~VARY    4  71   35,0~~       DESIGN CURRENT DENSITY                        (AMP/FTSQ)
 VARY    4  72    1,0       AREA OF A CELL                                (FTSQ)
 VARY    4  73   15,        NUMBER OF CELLS IN MODULE
~~VARY    4  75     1,17     VOLTAGE PER CELL                              (VOLTS)~~
 VARY    4  77    48,       RELATIVE HUMIDITY IN EXIT CATHODE STREAM
 VARY    4  78   95,        RELATIVE HUMIDITY IN EXIT ANODE GASES
 VARY    4  80    1,52      EXTERNAL WATER MAKEUP RATE TO MATRIX
 VARY    4  81    1,5       WEIGHT OF WATER PER CELL IN MATRIX,
 VARY    4  82    1,83      WEIGHT OF CS2CO3 IN CELL                      (LB)
~~VARY    4  83   55,        DESIRE SOLIDS CONCENTRATION IN MATRIX         (PER CENT)~~
 VARY    4  84   55,        ACTUAL SOLIDS CONCENTRATION IN MATRIX         (PER CENT)
 VARY    4  86   14,7       TOTAL PRESSURE OF STAGE                       (PSIA)
~~VARY    4  87   40,        THERMAL CAPACITANCE OF STAGE~~                  (BTU/F)
 VARY    4  92   33,0       HEAT XSFR CONDUCTANCE FROM COOLNT TO CELL (BTU/HR-F)
 VARY    4  94    0,        ADDITIONAL HEAT SOURCE/SINK TO MODULE         (BTU/HR)
~~ID**   34      DUMMY COMPONENT PROVIDING COOLANT FLOW TO COMPONENT 4  CARCL4~~
 KBAS   33        49                0  2
 VARY   33   1     100,     COOLANT FLOWRATE                              (LB/HR)
~~VARY   33   2     100,     TEMP OF COOLANT~~                               (F)
 VARY   33   3      20,     PRESSURE                                      (PSIA)
 VARY   33   4      20,     PRESSURE                                      (PSIA)
~~KBAS   34        49              33 0  2~~
 VARY   34   1     100,     COOLANT FLOWRATE                              (LB/HR)
 VARY   34   2     100,     TEMP OF COOLANT                               (F)
~~VARY   34   3      20,     PRESSURE~~                                      (PSIA)
 VARY   34   4      20,     PRESSURE                                      (PSIA)
 ID**    6       CONDENSING HEAT EXCHANGER H2O SEPARATOR SUBROUTINE ANYHX
~~KBAS    6        4              -3 2                     -36 0   2             7~~
 NSTR    6      211000100              LIQ,-GAS HX WITH PRI OUT TEMP CRITERIA FOR SIZ
 VARY    6  66     35,      OVERALL UA                                    (B/HR-F)
~~VARY    6  74     5,0      (NTU)MAX~~
 VARY    6  75     65,      DESIGN OUTLET TEMP PRI SIDE                   (F)
 VARY    6  76      3,      TOLERANCE FOR PRI SIDE TEMP                   (F)
5~~ID**   36      DUMMY COMPONENT PROVIDING COOLANT FLOW TO COMPONENT  9 6 HX~~
 KBAS   36        49                0  2
 VARY   36   1      40,     COOLANT FLOWRATE                              (LB/HR)
4~~VARY   36   2      45,     TEMP OF COOLANT~~                               (F)
 VARY   36   3      20,     PRESSURE                                      (PSIA)
 VARY   36   4      20,     PRESSURE                                      (PSIA)
3~~ID**    7      FLOW RETURN TO CABIN METERED,~~
 KBAS    7        29 12             6 2                                       8
 NSTR    7     1                       METER ALL CONSTITUENT FLOWS
2~~VARY    7  65     32,0     REFERENCE TEMP FOR ENTHALPY,~~                  (F)
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ID**     8       2ND STAGE CARBONATION CELL CO2 CONCENTRATION SYS. (CARCL2)
KBAS     8       25              -4 2                         2                 9
~~NSTR     8       01                         H2O BALANCE CONSTANT TEMP OF STAGE TRANSIENT~~
   Y     8  16            38      COMPONENT NUMBER OF COOLANT SUPPLY
VARY     8  54      70.0          AMBIENT GAS TEMP.                               (F)
~~VARY     8  55       0.1          CONDUCTANCE BETWEEN SURFACE AMBIENT GAS         (BTU/HR)~~
VARY     8  57      60.0          AMBIENT RADIATION WAL TEMPERATURE               (F)
VARY     8  58       2.0          THERMAL RADIATION FA FACTOR                     (FTSQ)
~~VARY     8  60      60.0          STRUCTURE TEMP FOR HEAT SHORTS                  (F)~~
VARY     8  61       0.1          CONDUCTANCE BETWEEN MODULE AND STRUCTURE        (BTU/HR-F)
VARY     8  65        .98         REMOVAL EFFICIENCY OF OXYGEN
VARY     8  67      172.          DESIRED MODULE TEMPERATURE.                     (F)
VARY     8  68      174.          HEATER TURNOFF TEMP.                            (F)
VARY     8  69      170.          HEATER TURNON TEMP                              (F)
~~VARY     8  70      172.          ACTUAL TEMP OF MODULE                           (F)~~
VARY     8  71       50.          DESIGN CURRENT DENSITY                          (AMP/FTSQ)
VARY     8  72       1.0          NUMBER OF CELLS IN MODULE
~~VARY     8  73       8.0          NUMBER OF CELLS IN MODULE~~
VARY     8  75       1.25         VOLTAGE PER CELL                                (VOLTS)
VARY     8  77       35.          RELATIVE HUMIDITY IN EXIT CATHODE GASSES
~~VARY     8  78       95.          RELATIVE HUMIFITY IN EXIT ANODE GASSES~~
VARY     8  80        .5          EXTERNAL H2O MAKEUP RATE I(R) IF NSTR1=1        (LB/HR)
VARY     8  81       1.20         WEIGHT OF H2O PER CELL IN MATRIX                (LB)
~~VARY     8  82       1.2          WEIGHT OF H3PO4 PER CELL IN MATRIX              (LB)~~
VARY     8  83       50.          DESIRED H3PO4 CONCENTRATION IN MATRIX
VARY     8  84       50.          ACTUAL H3PO4 CONCENTRATION IN MATRIX
~~VARY     8  85       6.0          VAPOR PRESSURE OF WATER OVER ELECTROLYTE        (PSIA)~~
VARY     8  86      14.7          TOTAL PRESSURE OF STAGE                         (PSIA)
 ARY     8  87       45.          THERMAL CAPACITANCE OF STAGE                    (BTU/F)
  RY     8  92       20.          HEAT TRNSFR CNDCTNC FROM COOLANT TO CELL        (B/HR-F)
VARY     8  94        0.          ADDITIONAL HEAT SOURCE/SINK TO MODULE           (BTU/HR)
ID**    38       DUMMY CONPONENT PROVIDING COOLANT FLOW TO COMPONENT 8  CARCL2
~~KBAS    38       49                 33 0    2~~
NSTR    38    1                          DUMMY COMPONENT PROVIDING COOLNT FLO TO CARCL2
VARY    38   1     100.           COOLANT FLOWRATE                                (LB/HR)
~~VARY    38   2     100.           TEMP                                            (F)~~
VARY    38   3      20.           PRESS                                           (PSI)
VARY    38   4      20.           PRESS                                           (PSI)
~~ID**     9       CONDENSOR SEPARATOR SIMULATED BY ANYHX CO2/H2O SEPARATION~~
KBAS     9        4                8 2                   -39 0                  10
NSTR     9       211000100                   LIQ.GAS HX WITH PRI OUT  TEMP CRITERIA FOR SIZ
~~VARY     9  66       1.5          OVERALL UA                                      BTU/HR-F~~
VARY     9  74       5.0          NTU(MAX)
VARY     9  75       45.          DESIGN OUTLET TEMP PRI SIDE                     (F)
~~VARY     9  76       5.0          TOLERANCE FOR PRI SIDE TEMP                     (F)~~
ID**    39       DUMMY COMPONENT PROVIDING COOLANT FLOW TO COMPONENT  9 HY
KBAS    39       49                 0    2
VARY    39   1      20.0          COOLANT FLOWRATE                                (LB/HR)
VARY    39   2      40.0          TEMP OF COOLANT                                 (F)
VARY    39   3      20.           PRESSURE                                        (PSIA)
~~VARY    39   4      20.           PRESSURE                                        (PSIA)~~
ID**    10       CONDENSOR SEPARATOR SIMULATED BY ANYHX O2/H2O SEPARATION
KBAS    10        4               -8 2                   -40 0                  20
~~NSTR    10       211000100                   LIQ-GAS HX WITH PRI OUT TEMP CRITERIA FOR SIZW~~
 ARY    10  66       3.0          OVERALL UA                                      (BTU/HR-F)
VARY    10  74       6.0          NTN(MAX)
~~VARY    10  75       45.          DESIGN OUTLET TEMP PRI SIDE                     (F)~~
VARY    10  76        5.          TOLERANCE FOR PRI SIDE TEMP                     (F)
ID**    40       DUMMY COMPONENT PROVIDING COOLANT FLOW TO COMPONENT 10 HX
~~KBAS    40       49                 0    2~~
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  VARY   40   1    10,0         FLOWRATE                                    (L2/HR)
  VARY   40   2    40,0         TEMPERATURE                                 (F)
~~VARY   40   3    20,0         PRESSURE                                    PSI~~
  VARY   40   4    20,0         PRESSURE                                    PSI
  ID**   20      COMPRESSOR SIMULATED BY FAN FOR STORING CO2 INTO THE RESERVOIR
~~KBAS   20      23             9 2                                         21~~
  NSTR   20       3                        CO2 COMPRESSOR FOR CO2 ACCU, ADD HEAT ONLY,
  ID**   21      CO2 RESERVOIR SIMULATED BY TANKG
~~KBAS   21      30             20 2                                        22~~
  NSTR   21     1100
  VARY   21  54    70,0         AMBIENT GAS TEMP                            (F)
  VARY   21  55      ,05        THERMAL CONDUCTAHCE BETWEEN SURFACE/AMBNT   (BTU/HR-F)
  VARY   21  57    60,          AMBIENT WALL TEMP                           (F)
  VARY   21  58     6,0         RADIATION FA FACTOR                         (FTSQ)
~~VARY   21  60     60,         STRUCTURE TEMP,                             (F)~~
  VARY   21  61     2,2         CONDUCTANCE BETWEEN TNK WALL AND STRUCT,    (BTN/HR-F)
  VARY   21  67    0,076        TOTAL WEIGHT IN TNK CO2                     (LBS)
~~VARY   21  68    80,0         DLUID TEMP IN TNK CO2                       (F)~~
  VARY   21  69     1,0         VOLUME                                      FTCUB
  VARY   21  70    10,0         CO2 PRESS                                   PSIA
~~VARY   21  71     ,076        WEIGHT OF NON CONDENSABLES IN TNK           (LB)~~
  VARY   21  74     ,205        SPECIFIC HEAT                               BTU/LB-F
  VARY   21  75    44,          MOLECULAR WEIGHT OF CO2                     LB/MOLE
~~VARY   21  78     ,076        WEIGHT OF CO2 IN TNK                        LB~~
  VARY   21  90    2,5          THERMAL CAPACITANCE OF TNK SHELL            (BTU/F)
  VARY   21  92     ,5          CONDUCTANCE BETWEEN FLUID AND WALL          (BTU/HR-F)
~~ID**   22      COMPRESSOR FOR STORING THE O2 INTO THE O2 RESERVOIR~~
  KBAS   22      23             10 2                                        23
  NSTR   22       3                        O2 COMPRESSOR FOR O2 ACCU ADD HEAT ONLY,
  ID**   23      O2 RESERVOIR SIMULATED BY TANKG
  KBAS   23      30             22 2                                        16
  NSTR   23     1100
~~VARY   23  54    70,0         AMBIENT GAS TEMP                            (F)~~
  VARY   23  55      ,05        THERMAL CONDUCTAHCE BETWEEN SURFACE/AMBNT   (BTU/HR-F)
  VARY   23  57    60,          AMBIENT WALL TEMP                           (F)
~~VARY   23  58     6,0         RADIATION FA FACTOR                         (FTSQ)~~
  VARY   23  60      60,        STRUCTURE TEMP,                             (F)
  VARY   23  61     2,2         CONDUCTANCE BETWEEN TNK WALL AND STRUCT,    (BTN/HR-F)
~~VARY   23  67    ,0555        TOTAL WEIGHT IN TNK O2                      (LBS)~~
  VARY   23  68    80,0         O2 TEMP IN TNK,                             (F)
  VARY   23  69     1,0         VOLUME                                      FTCUB
~~VARY   23  70    10,0         O2 PRESS                                    PSIA~~
  VARY   23  71     ,0555       WEIGHT OF NON CONDENSABLES IN TNK           (LB)
  VARY   23  74     ,217        SPECIFIC HEAT                               BTU/LB-F
~~VARY   23  75    32,          MOLECULAR WEIGHT OF O2                      LB/MOLE~~
  VARY   23  76     ,0555       WEIGHT OF O2 IN TNK                         LB
  VARY   23  90    2,5          THERMAL CAPACITANCE OF TNK SHELL            (BTU/F)
~~VARY   23  92     ,5          CONDUCTANCE BETWEEN FLUID AND WALL          (BTU/HR-F)~~
  ID**   16      H2O COLLECTOR FOR CONDENSATE THAT MAY BE FORMED
  KBAS   16      12              0  2                                       17
5 ~~KARY 16  16                5   COND~~
  KARY   16  17                6   CONDENSATE FROM HUMIDITY CONTROLLER
  KARY   16  18                9   CONDENSATE FROM CO2/H2O SEPARATOR
4 ~~KARY 16  19               10   CONDENSATE FROM H2O/O2 SEPARATOR~~
  ID**   17      PUMP FORCING CONDENSATE INTO H2O RESERVOIR
  KBAS   17      22             16 0   2                                    18
3 ~~NSTR 17     0002                       ADD HEAT TO FLUID STREAM NO OP OR PERFRMNC CAL~~
  ID**   18      H2O RESERVOIR SIMULATED BY TANKG
  KBAS   18      30             17 0   2                                    2
2 ~~NSTR 18     1200~~
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VARY  18  54    70,         AMBIENT GAS TEMP,
VARY  18  55      ,1        THERMAL CONDUCTANCE BETWEEN SURFAC AND AMB(BTU/HR-F)
~~VARY  18  57    60,         AMBIENT WALL TEMP,                          (F)~~
[illegible]RY  18  58     6,         RADIATION FA FACTOR                         (FTSQ)
VARY  18  60    60,         STRUCTURE TEMP,                             (F)
~~VARY  18  61      ,1        CONDUCTANCE STRUCTURE TO TNK                (BTU/HR-F)~~
VARY  18  67      62,4      TOTAL FLUID WEIGT IN INK                          (LB)
VARY  18  68      60,       FLUID TEMP IN INK                                  (F)
~~VARY  18  69      1,        FLUID VOLUME IN INK    (LB/FT CU)~~
VARY  18  70    14,7        PRESSURE IN INK                    (PSI)
VARY  18  72      62,4      WEIGHT OF LIQUID IN INK    (LB)
~~VARY  18  86      1,0       SPECIFIC HEAT~~                               (BTU/LB-F)
VARY  18  90      2,5       THERMAL CAPACITANCE OF TNK SHELL            (BTU/LB)
PLOT       7  20        0,     100,     PER CENT CO2 IN ANODE GAS - STAGE 1
~~PLOT       7  21        0,     100,     PER CENT CO2 IN CATHODE GAS - STAGE 1~~
PLOT       2  12                        CO2 IN PROCESS GAS TO SUBSYSTEM   LB/HR
PLOT       4  12                        CO2 IN PROCESS GAS LEAVING SUBSYSTEM LB/HR
PLOT       4  24                        CO2 + O2 GAS LEAVING ANODE STAGE 1 LB/HR
PLOT       7  22                        CO2 + O2 GAS LEAVING CATHODE STAGE 1 LB/HR
PLOT       8  12                        CO2 FROM STAGE2 CATHODE TO CO2 RES, LB/HR
~~PLOT       2   6                        WATER VAPOR IN PROCESS GAS   LB/HR~~
PLOT       8  29                        O2 FROM STAGE2 ANODE TO O2 RESRVR,  LB/HR
PLOT      20   6                        H2O IN CO2 TO CO2 TANK LB/HR
~~PLOT      22   6                        H2O IN O2  TO O2 TANK  LB/HR~~
PLOT      18   1                        H2O FROM WATER SUPPLY  LB/HR
ENDC
~~ENDR~~
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TAPE
BASIC            1       12        10        11     YEA        NAY
CASE        HYRDROGEN DEPOLARIZED CELL SAMPLE PROBLEM
$CASE1
      KCHOUT=0, KPRNT= 6, KPTINV(1)=006, KRUN=1,
      TMIN=-460., TMAX=4000., WTMAX=10000.,
      DTIME=10., START=0.,TIMEMX=1200., MAXSSI=4,
      MAXSLP=1,
      MINSSI=3 $
 $PROP1
      CPCO2=.197, CPDIL=.24, VISGAS=.045, WTMTC=16., CPTC=1.,
      XKGAS=.0147, WTMDIL=28., WTMCON=18., CPCONV=.44,
      CPCONL=1., CPOXY=.22,
      CP(1)=1., RHO(1)=62.4, VISC(1)= 2.22   ,WTM(1)=18., XK(1)=.350 ,
      CP(2)=3.41, RHO(2)=.0052, VISC(2)=.0216, WTM(2)=2., XK(2)=.106 $
ID**    1      SOURCE OF CABIN AIR FLOW
KBAS    1      49                3
VARY   01  01 1085.5             TOTAL FLOW TO SUBSYSTEM             (LB/HR)
VARY   01  02 75.                TEMPERATURE                         (F)
VARY   01  03 14.7               PRESSURE                            (PSIA)
VARY   01  04 14.7               PRESSURE                            (PSIA)
VARY   01  05 989.97             NON- CONDENSABLES                   (LB/HR)
VARY   01  06 9.4                H2O                                 (LB/HR)
VARY   01  10 228.               O2                                  (LB/HR)
VARY   01  11 756.               N2                                  (LB/HR)
VARY   01  12 5.973              CO2                                 (LB/HR)
VARY   01  13 .0001              TRACE CONTAMINATES                  (LB/HR)
ID**    2      HUMIDITY CONTROL HEAT EXCHANGER
NSTR    2      0110001           1
 BAS    2        4             1 3              -11 0   1                  3
VARY    2  66 50.                OVERALL UA                          (BTU/HR-F)
VARY    2  67 .95                EFFECTIVENESS                       (DIM)
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VARY    2  75 40,               DESIGN TEMPERATURE             (F)
ID**    3     SUBSYSTEM BLOWER
KBAS    3     23              2 3                                            4
NSTR    3      3
VARY    3  91 20,               HEAT DISS, INTO GAS            (WATTS)
ID**    4     BYPASS VALVE
KBAS    4     10              3 3                  3                         8
NSTR    4    0
VARY    4  65 0,00001           SPLIT RATIO                    (DIM)
ID**    5     HYRDROGEN DEPOLARIZED CELL MODULE
KBAS    5     32              4 3                =9 3  2                     6
KARY    5  16            1
KARY    5  17            2
KARY    5  18            3
KARY    5  19            4
KARY    5  20            5
KARY    5  21            6
KARY    5  22            7
VARY    5  65 3,0               MAXIMUM CO2 PARTIAL PRESSURE CABIN(MM HG)
VARY    5  66 62,0              CELL TEMPERATURE AT TIME ZERO  (F)
VARY    5  67 52,0              LOWEST AIR TEMP, FOR OPERATION (F)
VARY    5  68 14,7              MAXIMUM AIR PRESSURE FOR OPERAT,(F)
VARY    5  69 200,              MAXIMUM AIR FLOW FOR OPERATION (CFM)
VARY    5  70 7,925             MAXIMUM AIR WATER VAPOR PP     (MM HG)
VARY    5  71 0,5               CELL LENGTH                    (FT)
VARY    5  72 54,               TOTAL WIDTH OF ALL CELLS       (FT)
VARY    5  73 0,2               AIR CHANNEL DIMENSION          (INCHES)
VARY    5  74 0,05              CURRENT COLLECTOR WIDTH        (INCHES)
VARY    5  75 25,               ELECTRODE SPACING              (MILS)
VARY    5  76 60,               MATRIX THICKNESS BEFORE COMP,  (MILS)
VARY    5  77 0,70              MATRIX VOID VOLUME FRACTION    (DIM)
VARY    5  78 111,              TOTAL MASS OF CELL STACK       (LB)
VARY    5  79 ,125              AVERAGE CP OF CELL STACK       (BTU/LB=F)
VARY    5  80 6,1               AVAILABLE SPONGE VOL,OF MATRIX (ML/SQ FT)
VARY    5 129 1,
ID**    6     GAS MIX
KBAS    6      6              5 3                 4 3                        7
NSTR    6
ID**    7     FILTER
KBAS    7     11              6 3                                           10
NSTR    7    3
VARY    7  77 ,01               (1,= REMOVAL EFFICIENCY)       (DIM)
VARY    7  78
ID**    8     H2 STORAGE TANK
KBAS    8     30             12 3  2                                         9
NSTR    8    0210
VARY    8  54 75,               AMBIENT TEMPERATURE            (F)
VARY    8  55 2,                UA TO SURROUNDINGS             (BTU/HR=F)
VARY    8  67 0,014             INITIAL MASS(TOTAL)            (LB)
VARY    8  69 2,                TANK VOLUME                    (CU FT)
VARY    8  70 20,               INITIAL PRESSURE               (PSIA)
VARY    8  71 0,014             INITIAL MASS(NON= CONDENSABLES) (LB)
VARY    8  75 2,                MOLECULAR WEIGHT               (LB/LB MOLE)
VARY    8  80 0,014             INITIAL MASS H2                (LB)
VARY    8  68 75,               INITIAL TEMPERATURE            (F)
ID**    9     FILTER
KBAS    9     11              8 3  2                                         5
NSTR    9    3
VARY    9  77 ,01               (1,= REMOVAL EFFICIENCY)       (DIM)
VARY    9  78
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ID**  10       CO2/H2 ACCUMULATOR TANK
KBAS  10       30               -5 3   2                                    2
NSTR  10        0210
VARY  10  54 75,                AMBIENT TEMPERATURE                (F)
VARY  10  55 2,                 UA TO SURROUNDINGS                 (BTU/HR-F)
VARY  10  67 0,076              INITIAL MASS(TOTAL)                (LB)
VARY  10  68 75,                INITIAL TEMPERATURE                (F)
VARY  10  69 2,                 TANK VOLUME                        (CU FT)
VARY  10  70 20,                INITIAL PRESSURE                   (PSIA)
VARY  10  71 0,076              INITIAL MASS(NON CONDENSABLES)     (LB)
VARY  10  75 2,                 MOLECULAR WEIGHT                   (LB/LB MOLE)
VARY  10  78 0,062              INITIAL MASS CO2                   (LB)
VARY  10  80 0,014              INITIAL MASS H2                    (LB)
ID**  11       SOURCE OF COOLANT
KBAS  11       49                0   1
VARY  11  01 150,               TOTAL FLOW                         (LB/HR)
VARY  11  02 40,                TEMPERATURE                        (F)
VARY  11  03 14,7               PRESSURE                           (PSIA)
VARY  11  04 14,7               PRESSURE                           (PSIA)
ID**  12       SOURCE OF HYDROGEN
KBAS  12       49                3   2
VARY  12  01 0,182              HYDROGEN FLOW TO SUBSYSTEM         (LB/HR)
VARY  12  02 75,                TEMPERATURE                        (F)
VARY  12  03 14,7               PRESSURE                           (PSIA)
VARY  12  04 14,7               PRESSURE                           (PSIA)
VARY  12  05 0,182              NON- CONDENSABLES                  (LB/HR)
VARY  12  06 0,0001             WATER VAPOR                        (LB/HR)
VARY  12  13 ,001
VARY  12  14 0,182              H2                                 (LB/HR)
VARY  12  13 0,0001             TRACE CONTAMINATES                 (LB/HR)
TABL   1  1   3                 9     5    LIN   LIN   LIN
TITL   1  2 WATER VAPOR PRESSURE(MM HG) VS, CONC,(PERCENT) AND  TEMP,(F)
VALU   1 10 3I              45,         60,         70,         80,         90,
VALU   1 11 3D 0,           7,7         13,25       18,76       26,10       36,20
VALU   1 12 3D 40,          7,1         12,30       17,30       24,20       33,70
VALU   1 13 3D 50,          6,4         11,20       15,70       22,20       30,60
VALU   1 14 3D 60,          5,52        9,55        13,50       19,00       26,20
VALU   1 15 3D 65,          4,83        8,36        11,70       16,50       23,00
VALU   1 16 3D 70,          4,02        6,88        9,80        13,60       19,00
VALU   1 17 3D 73,          3,42        5,88        8,30        11,50       16,00
VALU   1 18 3D 75,          2,83        4,82        6,82        9,45        13,00
VALU   1 19 3D 77,          2,38        4,02        5,70        7,85        10,70
TABL   2  1   3                 9     5    LIN   LIN   LIN
TITL   2  2 CONC,(PER CENT) VS, TEMP,(F) AND H2O PARTIAL PRESS,(MM HG)
VALU   2 10 3I              ,9163       1,386       1,946       2,303       2,708
VALU   2 11 3D 45,          76,5        70,         41,40       0,          0,
VALU   2 12 3D 50,          78,3        73,3        57,0        0,          0,
VALU   2 13 3D 55,          80,         75,14       65,0        42,0        0,
VALU   2 14 3D 60,          80,         77,         69,65       57,0        0,
VALU   2 15 3D 65,          80,         78,75       73,0        65,         24,
VALU   2 16 3D 70,          80,         80,         74,74       69,5        53,0
VALU   2 17 3D 75,          80,         80,         76,54       72,70       62,5
VALU   2 18 3D 80,          80,         80,         79,70       74,30       67,5
VALU   2 19 3D 85,          80,         80,         80,         75,70       71,0
TABL   3  1   3                 9     5    LIN   LIN   LIN
TITL   3  2 SPECIFIC COND,(1,/OHM-CM) VS TEMP(F) AND CONC,(PERCENT)
VALU   3 10 3I              40,         50,         60,         71,         75,
VALU   3 11 3D 45,          ,144        ,170        ,165        ,104        .104
VALU   3 12 3D 50,          ,154        ,18         ,175        ,115        .115
VALU   3 13 3D 55,          ,163        ,191        ,185        ,125        .118
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VALU    3 14 3D 60.          .173         .201         .196         .136         .128
VALU    3 15 3D 65.          .183         .212         .206         .146         .138
VALU    3 16 3D 70.          .192         .222         .2170        .156         .138
VALU    3 17 3D 75.          .202         .233         .227         .167         .147
VALU    3 18 3D 80.          .211         .243         .238         .177         .144
VALU    3 19 3D 85.          .221         .253         .248         .187         .154
TABL    4  1    2            7            LIN   LIN
TITL    4  2 ELECTROLYTE CONCEN.(WT PER CENT) VS. MOLARITY(GMOLES/LITER)
VALU    4 10 2I 1.0          2.0          3.0          4.0          5.0          6.0
VALU    4 11 2D 25.          42.          54.5         63.0         69.5         74.5
VALU    4 12 2I 7.
VALU    4 13 2D 79.
TABL    5  1    2            7            LIN   LIN
TITL    5  2 ELECTROLYTE MOLARITY(GMOES/LITER) VS. CONCEN.(WT PER CENT)
VALU    5 10 2I 20.          30.          40.          50.          60.          70.
VALU    5 11 2D .7           1.25         1.87         2.60         3.6          5.05
VALU    5 12 2I 80.
VALU    5 13 2D 7.15
TABL    6  1    2            9            LIN   LIN
TITL    6  2 ELECTROLYTE SP. VOL(CM**3/GRAM) VS. CONCEN.(WT PER CENT)
VALU    6 10 2I 40.          45.          50.          55.          60.          65.
VALU    6 11 2D 1.667        1.4          1.176        .994         .847         .713
VALU    6 12 2I 70.          75.          80.
VALU    6 13 2D .606         .513         .45
TABL    7  1    2            10           LOG   LOG
TITL    7  2 REYNOLDS FACTOR VERSUS FRICTION FACTOR
VALU    7 10 2I 5.3    E-2 9.65   E-2 1.413  E-1 2.605  E-1 3.4    E-1 4.61   E-1
VALU    7 11 2D 2.05   E-4 8.3    E-4 1.805  E-3 5.35   E-3 8.38   E-3 1.373  E-2
VALU    7 12 2I 5.47   E-1 6.59   E-1 1.028      1.538
VALU    7 13 2D 1.788  E-2 2.368  E-2 4.488  E-2 7.6    E-2
PLOT         5 128  0.          1.          CO2 REMOVAL RATE(LB/HR)
PLOT         5  87  0.          1000.       TOTAL CURRENT(AMPS)
PLOT         5  85  0.          100.        AVERAGE CELL TEMPERATURE(F)
PLOT         5  98  0.          5.          CO2 IN AIR LEAVING CELL(MM HG)
PLOT         5  99  0.          20.         H2O IN AIR LEAVING CELL(MM HG)
PLOT         5 115                          CATHOLYTE CONCENTRATION(WT PERCENT)
PLOT         5 111  0.          2000.       HEAT GENERATED IN STACK(BTU/HR)
PLOT         5 110  0.          .5          CELL VOLTAGE(VOLTS)
PLOT         5  94  0.          500.        H2 PARTIAL PRESSURE EXIT H2 STREAM(MM HG)
PLOT         5  95  0.          100.        CO2 PARTIAL PRESSURE EXIT H2 STM(MM HG)
PLOT         5  96  0.          50.         H2O PARTIAL PRESSURE EXIT H2 STM(MM HG)
ENDC
ENDR
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*INSERT,GPOLY2,21
C       ***************SOLID ELECTROLYTE**************************************
        IF( N.NE.8) RETURN
        CALL SV( R(14), I3,14 )
        CALL SV( R(01), I3, 1 )
        CALL SV( R(05), I3, 5 )
TAPE
BASIC              1        I4        11         6     YEA        NAY
CASE           SOLID ELECTROLYTE CO2 REDUCTION CONCEPT
 $CASE1
        KCHOUT=0, KPRNT=006, KPTINV(1)=006, KRUN=1,
        TMIN=-460., TMAX=2000., WTMAX=10000.,
        DTIME=10., START=0., TIMEMX=1200., MAXSSI= 5,
        MAXSLP=3,
        MINSSI=4 $
 $PROP1
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        CPCO2=,197, CPDIL=.22, VISGAS=,045, WTMTC=16.,
        XKGAS=,0147, WTMDIL=28., WTMCON=18., CPCONV=,44,
        CPCONL=1., CPOXY=,22,
        CP(1)= 3,51, RHO(1)=0,0019, VISC(1)=0,0416, XK(1)=0,208,WTM(1)=2.,
        CP(2)= ,2730,RHO(2)=0,0263, VISC(2)=0,084,XK(2)=,0322,WTM(2)=44,,S
  ID**    1      CO2 FEED TANK(ACCUMULATOR)
  NSTR    1     0210
  KBAS    1      30             14 2                                           2
  VARY   01  54 75,                AMBIENT GAS TEMPERATURE           (F)
  VARY   01  55 2,0                UA INSUL SURFACE/AMBIENT          (BTU/HR-F)
  VARY   01  64 0,                 INSULATION CONDUCTANCE            (BTU/HR-F)
  VARY   01  69 2,                 TANK VOLUME                       (CU FT)
  VARY    1  68 75,
  VARY   01  78 1,                 FRACTION CO2 IN TANK
  VARY    1  70 14,7
  ID**    2      SUBSYSTEM BLOWER
  KBAS    2      23              1 2                                           3
  NSTR    2     003
  VARY    2  91 2,0                BLOWER HEAT DISSIPATION            (WATTS)
  ID**    3      HUMIDIFIER
  NSTR    3
  KBAS    3       6              2 2                    -12 2                  4
  ID**    4      GAS MIX
  NSTR    4
  KBAS    4       6              3 3   1 2              -11 3   1 2            5
  ID**    5      SOLID ELECTROLYTE CELLS
  NSTR    5     00
  KBAS    5      51              4 3   1 2              -13 3   1 2            6
  KARY    5  16              7     NUMBER CELLS/STACK
  KARY    5  17             18     NUMBER STACKS/MODULE
  KARY    5  18              8     NUMBER MODULES/UNIT
  VARY    5  51 1652,              SHELL TEMPERATURE                 (F)
  VARY    5  54 75,                AMBIENT TEMPERATURE               (F)
  VARY    5  55 2,1                UA INSUL, SURFACE TO AMBIENT      (BTU/HR-F)
  VARY    5  57 75,                AMBIENT WALL TEMPERATURE           (F)
  VARY    5  58                    SCRIPT FAINSULATION SURFACE TO WALL
  VARY    5  64 0,222              INSULATION CONDUCTANCE            (BTU/HR-F)
  VARY    5  65 500,               HEATER DISSIPATION                (BTU/HR)
  VARY    5  67 135,               TOTAL CURRENT TO UNIT             (AMPS)
  VARY    5  72 0,81               O2 CURRENT EFFICIENCY             (FRACTION)
  VARY    5  74 0,175              H2 CURRENT EFFICIENCY             (FRACTION)
  VARY    5  76 0,614              CELL VOLTAGE EFFICIENCY           (VOLTS)
  VARY    5  80 0,01               CONVERGENCE TOLERANCE             (PERCENT)
  VARY    5  81 4,0                MOLULE THERMAL CAPACITANCE        (BTU/F)
  VARY    5  82 1652,              INITIAL TEMPERATURE(TRANSIENT)    (F)
  ID**    6      O2 ACCUMULATOR
  NSTR    6     0210
  KBAS    6      30             -5 3   1 2                                     7
  VARY   06  54 75,                AMBIENT GAS TEMPERATURE           (F)
  VARY   06  55 2,                 UA INSUL,SURFACE/AMBIENT          (BTU/HR-F)
  VARY   06  64 ,5                 INSULATION CONDUCTANCE            (BTU/HR-F)
  VARY   06  69 2,                 TANK VOLUME                       (CU FT)
  VARY    6  68 75,
  VARY    6  70 14,7
  VARY   06  78 1,                 FRACTION O2 IN TANK
  ID**    7      HYDROGEN SEPARATOR
  NSTR    7     1
  KBAS    7      55              5 3   1 2              -13 3   1 2            8
  KARY    7  16              1     NUMBER OF H2 SEPARATION CELLS
  VARY    7  54 75,                AMBIENT GAS TEMPERATURE           (F)
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VARY    7  55 0,1              UA INSUL, SUR, TO SURROUNDINGS  (BTU/HR-F)
VARY    7  57 75,              AMBIENT WALL TEMPERATURE        (F)
~~VARY    7  58                 SCRIPT FA AMBIENT WALL/INSUL,SURFACE~~
V  Y    7  64 0,1              INSULATION CONDUCTANCE          (BTU/HR-F)
VARY    7  65 1,48             MEMBRANE AREA                   (SQ FT)
VARY    7  66 ,005             MEMBRANE THICKNESS              (INCHES)
VARY    7  77 1,
VARY    7  71 5,18    E-4      H2 PERMEABILITY(CU FT/HR)(INCHES)/(SQ FT-MMHG)
~~VARY    7  91 1,               UA CELL/WALL(PRIMARY SIDE)      (BTU/HR-F)~~
VARY    7  92 1,               UA CELL/WALL(SECONDARY SIDE)    (BTU/HR-F)
VARY    7  93 100,             UA ACROSS MEMBRANE              (BTU/HR-F)
VARY    7 103 0,667            CELL LENGTH                     (FT)
VARY    7 104 0,2              CELL FRONTAL AREA(PRIMARY SIDE) (SQ FT)
VARY    7 105 1,      E-9      CELL FRONTAL AREA(SECONDARY SIDE)(SQ FT)
~~VARY    7 106 0,1              MODULE THERMAL CAPACITANCE      (BTU/F)~~
VARY    7 107 0,9              DT MULTIPLYING FACTOR
VARY    7 108 0,1              MINIMUM ALLOWABLE COMPUTING INT,(F)
ID**    8      VACUUM PUMP
NSTR    8    10
KBAS    8     28          -7 3  1 2                                   9
~~VARY    8  75 20,              DISCHARGE PRESSURE              (PSIA)~~
VARY    8  66 0,60             MOTOR EFFICIENCY                (DIM)
VARY    8  67 0,40             AERODYNAMIC EFFICIENCY          (DIM)
VARY    8  71 0,               FRACTION Q LOST TO AMBIENT      (DIM)
KARY    8  16           3      TABLE FOR VACUUM PUMP FLOW
ID**    9      H2 ACCUMULATOR
~~NSTR    9    0210~~
KBAS    9     30          8 3  1 2                                    10
VARY   09  54 75,              AMBIENT GAS TEMPERATURE         (F)
   Y   09  55 2,               UA INSUL,SURFACE/AMBIENT        (BTU/HR-F)
VARY   09  64 0,5              INSULATION CONDUCTANCE          (BTU/HR-F)
VARY    9  68 75,
~~VARY   09  69 2,               TANK VOLUME                     (CU FT)~~
VARY    9  70 14,7
VARY   09  80 1,               FRACTION H2 IN TANK
ID**   10      CARBON DEPOSITION REACTOR
NSTR   10
KBAS   10     50          7 3  1 2                                    11
~~VARY   10  51 986,             TEMPERATURE                     (F)~~
VARY   10  54 75,              AMBIENT GAS TEMPERATURE         (F)
VARY   10  55 3,0              UA INSULATION/SURROUNDINGS      (BTU/HR-F)
VARY   10  57 75,              AMBIENT WALL TEMPERATURE        (F)
VARY   10  58 0,6              SCRIPT F INSULATION/WALL        (SQ FT)
VARY   10  64 4,56             INSULATION CONDUCTANCE          (BTU/HR-F)
~~VARY   10  65 1000,            ELECTRICAL HEATER DISSIPATION   (BTU/HR)~~
VARY   10  67 ,212             CO CONVERSION                   (FRACTION)
VARY   10  68 0,0              H2 CONVERSION                    (FRACTION)
VARY   10  71 ,01              CONVERGENCE TOLERANCE            (PERCENT)
VARY   10  74 986,             INITIAL TEMPERATURE             (F)
VARY   10  73 2,               TOTAL THERMAL CAPACITANCE        (BTU/F)
~~ID**   11      RECYLE BLOWER~~
KBAS   11     23         10 3  1 2                                    1
NSTR   11    003
VARY   11  01 7,6616           RECYCLE FLOW(TOTAL)               (LB/HR)
  RY   11  02 986,                     TEMPERATURE               (F)
VARY   11  03 14,2                     PRESSURE                  (PSIA)
~~VARY   11  04 14,2                     PRESSURE                  (PSIA)~~
VARY   11  06 ,0595                    WATER VAPOR               (LB/HR)
VARY   11  07                          LIQUID WATER              (LB/HR)
VARY   11  10                          OXYGEN                    (LB/HR)
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VARY  11  11                              NITROGEN                    (LB/HR)
VARY  11  12 4,92                         CO2                         (LB/HR)
VARY  11  13                              TRACE CONTAMINATES          (LB/HR)
V   Y 11  14 0,0221                       H2                          (LB/HR)
VARY  11  15 2,66                         CO                          (LB/HR)
VARY  11  91 60,                  RECYCLE BLOWER HEAT DISSIPATION    (WATTS)
ID**  12      WATER FEED TANK
KBAS  12      49                  2
VARY  12  01 0,1232               WATER FLOW TO HUMIDIFIER            (LB/HR)
VARY  12  02 75,                  TEMP, FLOW TO HUMIDIFIER            (F)
VARY  12  03 14,7                 PRESSURE FLOW TO HUMIDIFIER         (PSIA)
VARY  12  04 14,7                 PRESSURE FLOW TO HUMIDIFIER         (PSIA)
VARY  12  05 ,0001
VARY  12  06 ,0001
VARY  12  07 0,1230               WATER FLOW TO HUMIDIFIER            (LB/HR)
ID**  13      DUMMY COMPONENT
KBAS  13      49                   3   1 2
VARY  13  01 0,0136               FLOW HYDROGEN TO ACCUMULATOR    (LB/HR)
VARY  13  02
VARY  13  03 14,7
VARY  13  04 14,7
VARY  13  05 0,0136
VARY  13  08 3,4
VARY  13  09 2,
VARY  13  14 0,0136
ID**  14      SOURCE OF CO2(FROM CONCENTRATOR)
KBAS  14      49                  2
VARY  14  01 ,54204               TOTAL FLOW TO SUBSYSTEM         (LB/HR)
   Y  14  02 75,                  TEMPERATURE                     (F)
  RY  14  03 14,22                PRESSURE                        (PSIA)
VARY  14  04 14,22                PRESSURE                        (PSIA)
VARY  14  05 ,54203               FLOW NON-CONDENSABLES           (LB/HR)
VARY  14  06 ,00001               FLOW WATER VAPOR                (LB/HR)
VARY  14  07                      FLOW ENTRAINED WATER            (LB/HR)
VARY  14  10 ,00001               FLOW OXYGEN                     (LB/HR)
VARY  14  11 ,00001               FLOW NITROGEN                   (LB/HR)
VARY  14  12 ,542                 FLOW CO2                         (LB/HR)
VARY  14  13 ,00001               FLOW TRACE CONTAMINATES          (LB/HR)
TABL   1   1    3               10      4    LOG    LOG    LIN
TITL   1   2 VACUUM PUMP FLOW CHARACTERISTICS(SMALL PUMPS)
VALU   1 11 3I                 7,          14,7        30,         50,
VALU   1 12 3D 1,              1,6         1,8         1,9         1,95
VALU   1 13 3D 2,              1,55        1,79        1,89        1,94
VALU   1 14 3D 5,              1,3         1,65        1,88        1,92
VALU   1 15 3D 7,              1,15        1,52        1,85        1,90
VALU   1 16 3D 10,             1,0         1,40        1,75        1,85
VALU   1 17 3D 20,             0,62        1,08        1,45        1,65
VALU   1 18 3D 42,             0,00001     0,65        0,94        1,2
VALU   1 19 3D 100,            0,00001     0,00001     0,18        0,5
VALU   1 20 3D 130,            0,00001     0,00001     0,00001     0,3
VALU   1 21 3D 150,            0,00001     0,00001     0,00001     0,00001
PLOT       14  12   0,          1,          CO2 FLOW TO SUBSYSTEM(LB/HR)
PLOT        5  29   0,          1,          O2 FLOW TO ACCUMULATOR(LB/HR)
PLOT       12  07   0,          0,5         H2O FLOW TO SUBSYSTEM(LB/HR)
  OT       05  51   0,          1500,       CELL MODULE TEMPERATURE(F)
PLOT       10  51   0,          1500,       REACTOR TEMPERATURE(F)
PLOT        8  14   0,          0,1         H2 FLOW TO ACCUMULATOR(LB/HR)
ENDC
ENDR
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*I GPOLY1,24
C     ****************LIQUID ABSORPTION***********************************
      IF(NPASS .LT. 15  .OR.  N .NE. 2) GO TO 100
      NPASS=0
      PCO2N=VV(9,65)
      PCO2N=PCO2N-1,
      CALL SV(PCO2N,9,65)
  100 CONTINUE
      IF(N .NE. 14) GO TO 14
      A(15)=A(1)
      R(1)=VV(9,72)
      R(15)=R(1)
   14 CONTINUE
      IF(N .NE. 8) GO TO 8
      R(65)=A(1)*CPA*(185,-A(2))
      R(66)=185,
    8 CONTINUE
*I GPOLY2,21
      IF(N .NE. 4)  GO TO 4
      DO 40 KK=24,33
   40 R(KK)=0,
    4 CONTINUE
      IF(N .NE. 16) GO TO 16
      R(3)=14,7
      R(4)=14,7
   16 CONTINUE
      IF(N .NE. 18) GO TO 18
      R(3)=14,7
      R(4)=14,7
   18 CONTINUE
TAPE
BASIC           1       35        15        12      YEA        NAY
CASE         CO2 CONCENTRATOR USING LIQUID ABSORPTION
 $CASE1
  KCHOUT=0, KPRNT=6, KPTINV(1)=15,MAXSLP=4, MINSSI=2, KRUN=1, DTIME=30.,
  TIMEMX=4050,,MAXSSI=6, TMAX=250,,TMIN=-450,,WTMAX=1,E4 $
 $PROP1
  CPCONL=1,, CPCONV=0,44, CPCO2=0,2, CPDIL=0,25, CPOXY=0,22, CPTC=0,2,
 CP(1)=1,       ,CP(2)=,239     ,CP(5)=1,        ,CP(6)=,216      ,CP(7)=,28        ,
 RHO(1)=62,4   ,RHO(2)=,16     ,RHO(5)=62,4     ,RHO(6)=142,8    ,RHO(7)=136.      ,
 VISC(1)=3,6   ,VISC(2)=,036   ,VISC(5)=3,6     ,VISC(6)=3,6     ,VISC(7)=3,6      ,
 WTM(1)=18,    ,WTM(2)=28,     ,WTM(5)=18,      ,WTM(6)=138,2    ,WTM(7)=100.1     ,
 XK(1)=,235    ,XK(2)=,007     ,XK(5)=,325      ,XK(6)=,65       ,XK(7)=,65        ,
  GAMGAS=1,4, VISGAS=0,44, WTMCON=18,, WTMDIL=28,, WTMTC=20,,
  CPCO2 = ,178,        WTMCON=18, ,
  XKGAS=0,146 $
ID**     1    1 THIS COMPONENT DEFINES THE FLOW INTO THE CO2 CONCENTRATOR SYSTEM US
ID**     1    2 THE LIQUID ABSORPTION CONCEPT
KBAS     1      49                2
NSTR     1                               DUMMY COMPONENT DEFINING INLET FLOW TO CO2 CNT
VARY     1    1 368,283            TOTAL FLOW                                LB/HR
VARY     1    2 70,                TEMPERATURE                               F
VARY     1    3 14,7               UPSTREAM DUCT OUTLET PRESSURE             PSI
VARY     1    4 14,7               COMPONENT OUTLET PRESSURE                 PSI
VARY     1    5 364,201            NON-CONDENSABLE FLOW                      LB/HR
VARY     1    6 4,082              VAPOR FLOW                                LB/HR
VARY     1    7 0,                 CONDENSABLE ENTRAINED LIQUID FLOW         LB/HR
VARY     1    8 ,24145             NON-CONDENSABLE SPECIFIC HEAT             BTU/LB-F
VARY     1    9 29,048             NON-CONDENSABLE MOLECULAR WEIGHT          LBS/MOLE
VARY     1   10 96,920             PXYGEN FLOW                               -C2/Q9
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VARY    1  11 265,08           DILUENT FLOW                                LB/HR
VARY    1  12 2,201            CO2 FLO                                     LB/HR
VARY    1  13 0,               TRACE CONTAMINANT FLOW                      LB/HR
VARY    1  14 0,               SPECIAL FLOW NO, 1                          LB/HR
ID**    2   1 BLOWER FORCING THE CABIN AIR THROUGH THE CO2 CONCENTRATOR
KBAS    2     23           1 2                                           3
NSTR    2     3                   ADD HEAT NO HEAD RISE OR FAN PERFORMANCE CHAR,
ID**    3   1 LIQUID CONTACTOR SIMULATED BY SUBROUTINE LIQCON THE CO2 GAS IN THE
ID**    3   2 STREAM IS REACTED WITH THE CARBONATE SOLUTION TO FORM BICARBONATE
KBAS    3     52           2 3    5 6 7     -15 4    5 6 7               4
NSTR    3    01                   THE PROGRAM COMPUTES REQUIRED SECONDARY FLOWS
VARY    3  65 ,233333          REMOVAL EFFICIENCY OF THE ABSORBER TARGET,
VARY    3  66 ,6               TARGET CO2 REMOVAL RATE                 L3/HR
VARY    3  67 ,37              FRACTION OF BASE THAT IS BICARBONATE FLOWING IN
VARY    3  68 1,               NORMILITY OF BARBONATE SOLUTION FLOWING IN
ID**    4   1 LIQUID GAS SEPARATOR SIMULATED BY SUBROUTINE SPLIT SPECIAL FLOW COM
ID**    4   2 PONENTS ARE DIRECTED TO THE SECONDARY FLOW
KBAS    4     10 12        3 3    5 6 7          3       5 6 7           5
NSTR    4    1                    CALCULATE EACH OUTLET CONSTITUENT FLOW
VARY    4  66 0,            72 SPLIT RATIO FOR GAS
VARY    4  73 1,            76 SPLIT RATIO FOR LIQUIDS
ID**    5   1 CABIN AIR DEW POINT AND TEMP CONTRAL HEAT EXCHANGER SIMULATED BY
ID**    5   2 SUBROUTINE ANYHX
KBAS    5      4           4 2                  -25 0   2                5
NSTR    5    210000100            COUNTERFLO HX NO SIZING
VARY    5  66 130,             UA                                          BTJ/HR-F
VARY    5  75 65,              DESIGN OUTLET TEMP PRIMARY SIDE             F
VARY    5  76 15,              TOLERANCE FOR DESIGN OUTLET TEMP            F
ID**    6   1 FLOW RETURN TO CABIN AS MEASURED BY FLOW METER SUBROUTINE FLOMET
KBAS    6     29 12        5 2                                           7
NSTR    6    1                    METERED ALL FLOWS
VARY    6  65 32,0             REFERENCE TEMPERATURE FOR ENTHALPY          F
ID**    7   1 REGENERATIVE HEAT EXCHANGER FOR HEATING THE SOLUTION USING MINIMUM
ID**    7   2 HEAT INPUT
KBAS    7      4          -4 4    5 6 7     -18 4    5 6 7               8
NSTR    7    210020000            LIQ-LIQ COUNTERFLO HX NO SIZING
VARY    7  66 1385,            UA OF THE REGENERATIVE HX                   BTJ/LB-F
VARY    7  75 175,             DESIGN OUTLET TEMP PRIMARY SIDE             F
ID**    8   1 FOR HEATING THE SOLUTION TO DESIRED LEVELS COMPENSATING FOR THE
ID**    8   2 INEFFICIENCY OF THE REGENERATIVE HEAT EXCHANGER
KBAS    8     49           7 4    5 6 7                                  9
NSTR    8    1                    MODIFY R(ARRAY)
VARY    8  65 700,             HEAT LOAD
VARY    8  66 185,             TEMP OF OUTLET FLUID
ID**    9   1 FLASH VAPORIZATION AS SIMULATED BY LQFLSH  THIS COMPONENT SIMULATE
ID**    9   2 THE REACTION OF BICARBONATE TO GENERATE CARBONATE SOLUTION +CO2 +H2
ID**    9   3 O AND SEPARATE THE GAS FROM LIQUID,
KBAS    9     56           8 4    5 6 7            2                    15
NSTR    9                         LQFLSH
VARY    9   1 215,604          TOTAL FLOW                                  LB/HR
VARY    9   2 185,             TEMPERATURE                                 (F)
VARY    9   3 3,98864          PRESSURE,UPSTREM DUCT                       PSI
VARY    9   4 3,98864          COMPONENT OUTLET PRESS                      PSI
VARY    9  15 198,030          WATER                                       LB/HR
VARY    9  16 9,52496          CARBONATE                                   LB/HR
VARY    9  17 8,04875          BICARBONATE                                 LB/HR
VARY    9  54 70,              AMBIENT GAS TEMPERATURE                     (F)
VARY    9  55 ,5               CONDUCTANCE BETWEEN SURFACE AND AMBIENT GAS,BTU/HR-F
VARY    9  57 60,              AMBIENT RADIATION WALL TEMP                 (F)
VARY    9  58 8,               RADIATION FA FACTOR FROM SURFACE TO WALL  (FTSQ)
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VARY    9  60 60.              STRUCTURE TEMPERATURE FOR HEAT SHORTS     (F)
VARY    9  61 .1               THERMAL CONDUCTANCE BETWEEN MODULE/STRUCTR BTU/HR-F
~~VARY    9  64 .3               CONDUCTANCE BETWEEN MODULE/SURFACE INSULATION B/HR-F~~
  RY    9  65 10.              CO2 PARTIAL PRESSURE IN VAPORIZER         MMHG
VARY    9  68 1.               DESIRED NORMALITY OF SOLUTION
VARY    9  80 1.               DESIRED NORMALITY OF SOLUTION
ID**   10   1 H20 CONDENSOR USED TO SEPARATE H20 FROM CO2 BY CONDENSATION (ANYHX)
KBAS   10      4           16 2                    -30 0   2               12
~~NSTR   10     200000100                HI3/CO2 CONDENSOR  LIQ-GAS COUNTERFLO HX NOSIZ~~
VARY   10  66 100.             UA                                        BTU/LB-F
VARY   10  75 50.              DESIGN OUTLE TEMP PRI SIDE                F
VARY   10  76 5.               TOLERANCE DESIGN TEMP                     F
ID**   12   1 THE CO2 GAS FLOWS INTO CO2 RESERVOIR SIMULATED BY TANKG
KBAS   12     30           10 2                                            13
~~NSTR   12     1100                     CO2 TNK TEMP SET~~
VARY   12  54 70.              AMBIENT GAS TEMP                          F
VARY   12  55 5.               THERMAL CONDUCTANCE BETWEEN AMBIENT TNK   BTU/HR-F
VARY   12  57 60.              AMBIENT WALL TEMP                         F
VARY   12  58 6.               REAIATION FA SKIN TO WALL                 FTSQ
VARY   12  60 60.              STRUCTURE TEMP                            F
~~VARY   12  61 12.              CONDUCTANCE BETWEEN TNK AND STRUCTURE     BTU/HR-F~~
VARY   12  67 0.5              TOTAL FLUID WEIGHT IN TNK                 LB
VARY   12  68 70.              FLUID TEMP IN TNK                         F
VARY   12  69 1.               FLUID VOLUME IN TNK                       FTCV
VARY   12  70 14.7             FLUID PRESS IN TNK                        PSI
VARY   12  71 0.5              WEIGHT OF NON-CONDENSABLE IN TNK          LBS
~~VARY   12  74 .17              NON CONDENSABLE SPECIFIC HEAT IN TNK      BTU/LB-F~~
VARY   12  75 44.              NON-CONDENSABLE MOLECULAR WEIGHT          LB/MOLE
VARY   12  78 0.5              WEIGHT OF CO2 IN TNK                      LB
   *   15   1 CHILLER TO COOL DOWN THE CARBONATE SOLUTION SIMULATED BY ANYHX,
KBAS   15      4           -7 4     5 6 7          -35 0   2                2
NSTR   15     210020000                LIQ-LIQ COUNTERFLO HX NO SIZING
~~VARY   15  66 142.             UA                                        BTU/HR-F~~
VARY   15  75 70.              DESIGN OUTLET TEMP                        F
ID**   13   1 THE CONDENSATE IS COLLECTED BY H20 COLLECTOR SIMULATED BY H2OSUM
KBAS   13     12              0   1                                        14
KARY   13  16              2   NUMBER OF COMPONENSATE IS COLLECTED FROM
KARY   13  17              5   FIRST COMPONENT CONTRIBUTING CONDENSATE
~~KARY   13  18             10   SECOND COMPONENT CONTRIBUTING CONDENSATE~~
VARY   13   3 14.7             COMPONENT PRESS
VARY   13   4 14.7             COMPONENT PRESS
ID**   14   1 H20 SUPPLY TANK (TANKG) RECEIVES THE CONDENSATE FROM 13 AND PROVIDE
ID**   14   2 S MAKEUP W20
KBAS   14     30           13 4     5 6 7                                  17
~~NSTR   14     1100                     WATER TNK ONLY PRAYER BUT GOD WORKS FOR NOBODY~~
VARY   14   1 5.8951           FLOW                                      LB/HR
VARY   14   2 70.              TEMP.                                     F
VARY   14   3 14.7             PRESS                                     PSI
VARY   14   4 14.7             PRESS                                     PSI
VARY   14  15 5.8951           FLOW                                      LB/HR
~~VARY   14  54 70.              AMBIENT GAS TEMP                          F~~
VARY   14  55 5.               CONDUCTANCE SURFACE INSULATION TO AMBIENT BTU/HR-F
VARY   14  57 60.              AMBIENT WALL TEMP                         F
VARY   14  58 6.               RADIATION FA FACTOR                       FISQ
  RY   14  60 60.              STRUCTUR TEMP                             F
VARY   14  64 .05              CONDUCTANCE BETWEEN WALL AND INSULATION   BTU/HR-F
~~VARY   14  67 62.4             TOTAL FLUID WEIGHT IN TNK                 LB~~
VARY   14  68 60.              FLUID TEMP IN TNK                         F
VARY   14  69 1.               FLUID VOLUME IN TNK                       CUFT
VARY   14  81 62.4             WEIGHT OF SPECIAL FLOW NO, 2 IN TANK
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VARY  14  92 5,0             MAX  ALLOWABLE TEMP CHANGE FOR SS             F
ID**  16     VACUUM PUMP SIMULATED BY FAN TO PUMP OUT CO2/H2O GAS FROM LOFLSH
KBAS  16     23            -9 2                                            10
  TR  16      3                    ADD HEAT SPECIFIED ONLY NO HEAD  RISE/PERFORMN
ID**  17     JUNCTION WHICH PROVIDES FOR THE ADDITION OR MAKEUP WATER TO SYSTEM
KBAS  17      7             9 4      5 6 7       -14 4    5 6 7            18
NSTR  17    1                      OUTLET PRESS EQUALS PRIMARY SOURCE
ID**  18     WATER PUMP WHICH REMOVES AND PRESSURIZED THE WATER TO 1 ATM.
NSTR  18      2                    ADD HEAT ONLY NO HEAD RISE OR PUMP PERFORMANCE
KBAS  18     22            17 4      5 6 7                                 15
VARY  18   1 216,16          TOTAL FLOW                                    LB/HR
VARY  18   2 173,            TEMP,                                         F
VARY  18   3 14,7            PRESS,UPSTREAM DUCT                           PSI
VARY  18   4 14,7            PRESS,COMPONENT OUTLET                        PSI
VARY  18  15 199,990         H2O FLOW                                      LB/HR
VARY  18  16 8,5912          K2CO3 FLOW                                    LB/HR
VARY  18  17 7,57385         KHCO3 FLOW                                    LB/HR
ID**  25   1 DUMMY COMPONENT PROVIDING COOLNT FLOW TO COMPONENT NO, 5 .
KBAS  25     49              0   1
NSTR  25                           COOLANT TO CABIN TEMP/HUMIDT CONTROL
VARY  25   1 150,            COOLANT FLOW                                  LB/HR
VARY  25   2 45,             COOLANT TEMP                                  F
VARY  25   3 15,             PRESS, UPSTREAM DUCT                          PSIA
VARY  25   4 15,             PRESS, COMPONENT OUTLET                       PSIA
ID**  30   1 DUMMY COMPONENT PROVIDING COOLANT FLOW TO COMPONENT NO, 10,
KBAS  30     49              0   1
NSTR  30                           COOLANT TO H2O/CO2 SEPARATOR
VARY  30   1 250,            COOLANT FLOW                                  LB/HR
  ARY 30   2 35,             TEMPERATURE                                   F
   RY 30   3 10,             PRESSURE                                      PSI
VARY  30   4 10,             PRESSURE                                      PSI
ID**  35   1 DUMMY COMPONENT PROVIDING COOLANT FLOW TO COMPONENT NO, 15,
KBAS  35     49              0   1
NSTR  35                           COOLANT TO CHILLER
VARY  35   1 100,            COOLANT FLOW                                  LB/HR
VARY  35   2 45,             TEMP                                          F
VARY  35   3 10,             PRESS,                                        PSI
VARY  35   4 10,             PRESS,                                        PSI
PLOT       3  72   0,        10,        PPCO2 GAS FLOWING IN CO2 CONCENTRATOR MMHG
PLOT       3  69   0,        10,        PPCO2 GAS LEAVING CO2 CONCENTRATOR  -MMHG
PLOT       2   2   0,        100,       GAS TEMP ENTERING CO2 CONCENTRATOR DEG-F
PLOT       3   2   0,        100,       GAS TEMP LEAVING CO2 CONCENTRATOR  DEG-F
PLOT       9  65   0,        15,        PPCO2 IN FLASH VAPORIZATION MODULE MMHG
PLOT       9   4   0,        15,        TOTAL PRESSURE IN VAPORIZATION MODULE PSI
PLOT      15   1                        SOLUTION FLOW THROUGH CO2 CONCENTRTR LB/HR
PLOT       2   1                        GAS FLOWING THROUGH CO2 CONCENTRATOR LB/HR
PLOT       8  65                        HEAT ADDED PRIOR TO VAPORIZATION BTU/HR
PLOT       9  71                        HEAT ADDED TO THE VAPORIZER BTU/HR
PLOT      13   1                        TOTAL WATER CONDENSATED IN HX LB/HR
PLOT      14   1                        WATER ADDED TO THE SYSTEM LB/HR
ENDC
ENDR
*
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*INSERT,GPOLY1,24
C       ***************ELECTRODIALYSIS****************************************
        IF( N.NE.31) RETURN
        TOTAL MAKEUP WATER TO ELECTRODIALYSIS SUBSYSTEM
        WHUM=.55
        WTOT= VV(12,81)*WHUM
        IF(WTOT.LE.0.) GO TO 10
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      CALL SV(WTOT,3,1)
      CALL SV( WTOT,3,15)
C                SET FLOW TO HUMIDIFIER
      RH65= WHUM/WTOT
      IF( RH65,LT,0,) RH65= 0.
      IF(RH65,GT,1,) Rw65= 1.
      CALL SV( RH65,5,65)
      T1= VV(5,21)
      P1= VV(5,23)
      CALL SV(WHUM,27,90)
      CALL SV(WHUM,27,26)
      CALL SV(T1,27,21)
      CALL SV(P1,27,23)
      WTT= WTOT-WHUM
      IF( WTT,LE,0) GO TO 10
C                SET MAKEUP FLOW TO CATHODE LOOP
      WC= VV(12,83)
      R665= WC/WTT
      IF( R665,GT,1,) R665= 1.
      IF( R665,LT,0,) R665= 0.
      CALL SV( R665, 6, 65)
   10 CONTINUE
TAPE
BASIC            1      51      16      7    YEA      NAY
CASE        CO2 ELECTRODDALYSIS MODULE SAMPLE PROBLEM
 $CASE1
      KCHOUT=0, KPRNT=006, KPTINV(1)=006, KRUN=1,
      TMIN=-460,, TMAX=2000,, WTMAX=10000,,
      DTIME=10,, START=0,, TIMEMX=1200,, MAXSSI=5,,
      MAXSLP=3,
      MINSSI=3 $
 $PROP1
      CPCO2=,197, CPDIL=,25, VISGAS=,045, WTMTC=16,,
      XKGAS=,0147, WTMDIL=28,,WTMCON=18,, CPCONV=,44,
      CPCONL=1,, CPOXY=,22,
      CP(1)=1,0, RHO(1)=62,4, VISC(1)=2,22, XK(1)=,35, WTM(1)=18,,
      CP(2)=,22,RHO(2)=,0827,VISC(2)=,0492,XK(2)=,0152,WTM(2)=32,,
      CP(3)=3,41,RHO(3)=,0052,VISC(3)=,0216,XK(3)=,106,WTM(3)=2,,
      CP(4)=,198,RHO(4)=,114, VISC(4)=,0363,XK(4)=,0094,WTM(4)=44,, $
ID**   1      SOURCE OF FLOW TO SUBSYSTEM
KBAS   1      49            3
VARY   01  01 207,037        FLOW GAS FROM CABIN                   (LB/HR)
VARY   01  02 75,            TEMPERATURE                           (F)
VARY   01  04 14,7           PRESSURE                              (LB/SQ IN)
VARY   01  06 1,4            WATER VAPOR                           (LB/HR)
VARY   01  10 47,6           OXYGEN                                (LB/HR)
VARY   01  11 156,8          NITROGEN                              (LB/HR)
VARY   01  12 1,237          CARBON DIOXIDE                        (LB/HR)
VARY   01  13 ,0001          TRACE CONTAMINATES                    (LB/HR)
ID**   2      SOURCE OF SWEEP FLUID
KBAS   2      49            4     1 2 3 4
VARY   02  01 200,           SWEEP LIQUID FLOWRATE                 (LB/HR)
VARY   02  02 75,            TEMPERATURE                           (F)
VARY   02  04 14,7           PRESSURE                              (LB/SQ IN)
[illegible]RY   02  15 200,           WATER FLOWRATE                        (LB/HR)
ID**   3      WATER FEED TANK
KBAS   3      30            4     1 2 3 4                                      4
NSTR   3     1210
VARY   03  01 0,658          TOTAL FLOW OUT OF TANK                (LB/HR)
VARY   03  54 75,            AMBIENT TEMPERATURE                   (F)
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VARY   03   55 2.             UA TO SURROUNDINGS               (BTU/HR-F)
VARY   03   68 75.            GAS TEMPERATURE                  (F)
~~VARY   03   69 2.0            VOLUME LIQUID IN TANK            (CU FT)~~
   Y   03   70 14.7           PRESSURE                         (LB/SQ IN)
VARY   03   81 1.0            FRACTION WATER IN TANK           (FRACTION)
~~ID**    4      WATER MAKEUP TANK~~
KBAS    4      30              3 4    1 2 3 4                                5
NSTR    4     0210
~~VARY   04   01 0.658          TOTAL FLOW OUT OF TANK           (LB/HR)~~
VARY   04   54 75.            AMBIENT TEMPERATURE              (F)
VARY   04   55 2.             UA TO SURROUNDINGS               (BTU/HR-F)
VARY   04   68 75.            GAS TEMPERATURE                  (F)
VARY   04   69 .15            VOLUME LIQUID IN TANK            (CU FT)
VARY   04   70 14.7           PRESSURE                         (LB/SQ IN)
~~VARY   04   81 1.0            FRACTION WATER IN TANK           (FRACTION)~~
ID**    5      FLOW SPLIT
KBAS    5      10              4 4    1 2 3 4          4     1 2 3 4         6
VARY    5   65 0.             SPLIT RATIO
ID**    6      FLOW SPLIT
KBAS    6      10              5 4    1 2 3 4          4     1 2 3 4         12
~~VARY    6   65 0.666          SPLIT RATIO~~
ID**    7      SOURCE COOLANT TO CONDENSER 21
VARY   07   01 64.            FLOW COOLANT TO HX COMP. 21      (LB/HR)
VARY   07   02 50.0           TEMPERATURE                      (F)
VARY   07   04 14.7           PRESSURE                         (LB/SQ IN)
ID**    8      SOURCE COOLANT TO CONDENSER 24
~~VARY   08   01 150.           FLOW COOLANT TO HX COMP. 24      (LB/HR)~~
VARY   08   02 50.            TEMPERATURE                      (F)
KBAS    7      49               0   1
   S    8      49               0   1
KBAS    9      49               0   1
VARY   08   04 14.7           PRESSURE                         (LB/SQ IN)
~~ID**    9      SOURCE COOLANT TO CONDENSER 14~~
VARY    9   01 64.            TOTAL FLOW                       (LB/HR)
VARY    9   02 50.            TEMPERATURE                      (F)
VARY    9   04 14.7           PRESSURE                         (PSIA)
ID**   10      SUBSYSTEM BLOWER
KBAS   10      23              1 3                                           11
~~NSTR   10     003~~
VARY   10   91 50.            HEAT DISSIPATION                 (WATTS)
ID**   11      HUMIDIFIER
KBAS   11       6            10 3                      27 3                  3
NSTR   11     00
ID**   12      ELECTRODIALYSIS MODULE
~~KBAS   12      53            11 3                      -2 4     1 2 3 4        14~~
NSTR   12      2
KARY   12   16          13    ALTERNATE COMPONENT
KARY   12   17           2    NUMBER OF STACKS/MODULE
KARY   12   18          40    NUMBER OF CELL UNITS/STACK
VARY   12   51 75.            ESTIMATED MODULE TEMPERATURE     (F)
~~VARY   12   54 75.            AMBIENT GAS TEMPERATURE          (F)~~
VARY   12   55 6.             UA TO SURROUNDINGS               (BTU/HR-F)
VARY   12   57 75.            AMBIENT WALL TEMPERATURE         (F)
VARY   12   66 4.6            CURRENT DENSITY                  (AMPS/SQ FT)
  RY   12   67 0.72           AREA PER ANODE                   (SQ FT)
VARY   12   68 1.28           CURRENT EFFICIENCY               (FRACTION)
~~VARY   12   69 90.            RH PROCESS GAS EFFLUENT          (PER CENT)~~
VARY   12   71 212.           STACK VOLTAGE                    (VOLTS)
VARY   12   72 0.3            POWER EFFICIENCY                 (FRACTION)
VARY   12   74 75.            ESTIMATED MODULE TEMPERATURE     (F)
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VARY  12  75 1,00           CONVERGENCE TOLERANCE          (PER CENT)
VARY  12  84 18,            MODULE THERMAL CAPACITANCE     (BTU/F)
VARY  12  85 75,            MODULE INITIAL TEMPERATURE     (F)
   *  13     ALTERNATE COMPONENT(ELECTRODIALYSIS MODULE)
KBAS  13     49         20 4    1 2 3 4     -18 4    1 2 3 4
NSTR  13   0
ID**  14     HEAT EXCHANGER FOR CATHODE EFFLUENT
KBAS  14      4        -13 4    1 2 3 4     -9 0   1                 31
NSTR  14   0   2           1
VARY  14  01 64,            FLOW COOLANT TO HX COMP, 14    (LB/HR)
VARY  14  02 50,            TEMPERATURE                    (F)
VARY  14  04 14,7           PRESSURE                       (LB/SQ IN)
VARY  14  67 0,9            EFFECTIVENESS                  (FRACTION)
ID**  15     H2 COMPRESSOR
KBAS  15     23        -31 3    1 2 3 4                              16
NSTR  15   003
VARY  15  91 5,0            HEAT DISSIPATION               (WATTS)
ID**  16     H2 ACCUMULATOR
NSTR  16   0210
KBAS  16     30         15 3    1 2 3 4                              10
VARY  16  01 0,0216         H2 USE RATE                    (LB/HR)
VARY  16  02 75,            TEMPERATURE                    (F)
VARY  16  03 20,0           PRESSURE                       (LB/SQ IN)
VARY  16  04 20,0           PRESSURE                       (LB/SQ IN)
VARY  16  54 75,            AMBIENT TEMPERATURE            (F)
VARY  16  55 2,             UA TO SURROUNDINGS             (BTU/HR-F)
VARY  16  68 75,            GAS TEMPERATURE                (F)
VARY  16  69 2,             TANK VOLUME                    (CU FT)
  RY  16  70 20,0           GAS PRESSURE                   (LB/SQ IN)
  RY  16  83 1,             FRACTION HYDROGEN              (FRACTION)
ID**  17     FLOW MIX MAKEUP WATER CATHODE LOOP
KBAS  17      7         31 4    1 2 3 4       6 4    1 2 3 4         18
NSTR  17
ID**  18     CATHODE LOOP PUMP
KBAS  18     22         17 4    1 2 3 4                              24
NSTR  18       2
VARY  18  01 64,            CATHODE LOOP FLOW              (LB/HR)
VARY  18  02 50,            TEMPERATURE                    (F)
VARY  18  04 14,7           PRESSURE                       (LB/SQ IN)
VARY  18  15 64,            WATER FLOW                     (LB/HR)
VARY  18  85 10,            THERMAL DISSIPATION            (WATTS)
ID**  19     FLOW MIX MAKEUP WATER CATHODE LOOP
KBAS  19      7         29 4    1 2 3 4      -6 4    1 2 3 4         20
NSTR  19
ID**  20     ANODE LOOP PUMP
KBAS  20     22         19 4    1 2 3 4                              22
NSTR  20       2
VARY  20  01 64,            ANODE LOOP FLOW                (LB/HR)
VARY  20  02 50,            TEMPERATURE                    (F)
VARY  20  04 14,7           PRESSURE                       (LB/SQ IN)
VARY  20  15 64,            WATER FLOW                     (LB/HR)
VARY  20  85 10,            THERMAL DISSIPATION            (WATTS)
ID**  21     HEAT EXCHANGER FOR ANODE EFFLUENT
KBAS  21      4         13 4    1 2 3 4     -7 0   1                 29
   TR 21   0   2           1
VARY  21  67 0,9            EFFECTIVENESS                  (FRACTION)
ID**  22     O2 COMPRESSOR
KBAS  22     23        -29 3    1 2 3 4                              23
NSTR  22   003
VARY  22  91 5,0            HEAT DISSIPATION               (WATTS)
```

```
ID**  23      O2 ACCUMULATOR
KBAS  23      30             22 3      1 2 3 4                                     25
NSTR  23      0210
  RY  23  01 .17             O2 USE RATE                      (LB/HR)
VARY  23  54 75.             AMBIENT TEMPERATURE              (F)
VARY  23  55 2.              UA TO SURROUNDINGS               (BTU/HR-F)
VARY  23  68 75.             GAS TEMPERATURE                  (F)
VARY  23  69 2.              TANK VOLUME                      (CU FT)
VARY  23  70 20.             GAS PRESSURE                     (LB/SQ IN)
VARY  23  82 1.              FRACTION OXYGEN                  (FRACTION)
ID**  24      HEAT EXCHANGER FOR CONCENTRATOR EFFLUENT
KBAS  24      4             -12 4      1 2 3 4       -8 0   1                      30
NSTR  24    0   2            1
VARY  24  67 0.9             EFFECTIVENESS                    (FRACTION)
ID**  25      CO2 COMPRESSOR
KBAS  25      23            -30 3      1 2 3 4                                     26
NSTR  25     003
VARY  25  91 5.0             HEAT DISSIPATION                 (WATTS)
ID**  26      CO2 ACCUMULATOR
NSTR  26     0210
KBAS  26      30             25 3      1 2 3 4                                     15
VARY  26  54 75.             AMBIENT TEMPERATURE              (F)
VARY  26  55 2.              UA TO SURROUNDINGS               (BTU/HR-F)
VARY  26  68 75.             GAS TEMPERATURE                  (F)
VARY  26  69 2.              TANK VOLUME                      (CU FT)
VARY  26  70 20.             GAS PRESSURE                     (LB/SQ IN)
VARY  26  84 1.              FRACTION CARBON DIOXIDE          (FRACTION)
VARY  26  01 .575            CO2 USE RATE                     (LB/HR)
ID**  27      SOURCE LICUID FLOW TO HUMIDIFIER
  AS  27      49                                      3
VARY  27  20 0.55            LIQUID FLOW TO HUMIDIFIER        (LB/HR)
VARY  27  21 75.             TEMPERATURE                      (F)
VARY  27  23 14.7            PRESSURE                         (LB/SQ IN)
VARY  27  24 1.       E-6
VARY  27  25 1.       E-6
VARY  27  28 29.
VARY  27  26 0.55            LIQUID WATER                     (LB/HR)
ID**  29      O2/WATER SEPARATOR
KBAS  29      10  5          21 4      1 2 3 4        4     1 2 3 4                19
NSTR  29     1
VARY  29  67 0.9999          O2 SPLIT RATIO                   (FRACTION)
VARY  29  66 0.0001          WATER SPLIT RATIO                (FRACTION)
ID**  30      CO2/WATER SEPARATOR
KBAS  30      10  5          24 4      1 2 3 4        4     1 2 3 4                21
NSTR  30     1
VARY  30  66 0.0001          WATER SPLIT RATIO                (FRACTION)
VARY  30  69 0.9999          CO2 SPLIT RATIO                  (FRACTION)
ID**  31      H2/WATER SEPARATOR
KBAS  31      10  5          14 4      1 2 3 4        4     1 2 3 4                17
NSTR  31     1
VARY  31  68 0.9999          H2 SPLIT RATIO                   (FRACTION)
VARY  31  66 0.0001          WATER SPLIT RATIO                (FRACTION)
PLOT      10  12  0.         2.        CO2 IN PROCESS GAS ENTERING MODULE(LB/HR)
PLOT      12  12  0.         2.        CO2 IN PROCESS GAS LEAVING MODULE(LB/HR)
  OT      13  16  0.         .5        O2 GENERATED BY ELECTROLYSIS(LB/HR
  OT      13  36  0.         .5        H2 GENERATED BY ELECTROLYSIS(LB/HR)
PLOT      12  37  0.         .5        CO2 REMOVED IN MODULE(LB/HR)
PLOT      12  51  0.         100.      MODULE TEMPERATURE(F)
PLOT      12  81  0.         2.        TOTAL WATER CONSUMED(LB/HR)
ENDC
```

```
*INSERT,GPOLY2,21
C       ***************MOLTEN CARBONATE*************************************
        IF(.NOT.STEADY) GO TO 10
        IF( N.NE.5) RETURN
        TSET=1050.
        R65=VV(13,65)
        R65= R65 + (R(51)-TSET)/TSET *5.
        IF( R65.GT.1.0)  R65=1.
        IF( R65.LT.0.)  R65=0.
        CALL SV( R65, 13, 65)
        RETURN
     10 CONTINUE
        IF(N.NE.7) RETURN
        IF(NPASS.LE.0) RETURN
C       BYPASS FLOW CONTROLLED BY TEMPERATURE CONTROLLER
        R65= VV(10,68)
        CALL SV(R65,13,65)
C       ADJUST MOLTEN CARBONATE CELL TO CONTROL CO2 PARTIAL PRESSURE
        R67= VV(9,68)
        CALL SV(R67,5,67)
*INSERT,GPOLY1,24
        IF(STEADY) RETURN
        IF( N.EQ.9) GO TO 9
        IF( N.NE.10) RETURN
C       TEMPERATURE CONTROLLER
        TMP= VV(5,02)
        R(66)=TMP
        RETURN
C       CURRENT CONTROLLER
      9 CONTINUE
        PAIR= VV(5,04)
        WCO2= VV(5,12)
        XWT= VV(5,09)
        WAIR= VV(5,01)
        IF( WAIR.LE.0.)RETURN
        PCO2= WCO2*XWT*PAIR/ ( WAIR*44.)
        R(66)= PCO2
TAPE
BASIC           1       14       7        9     YEA       NAY
CASE          MOLTEN CARRONATE CONCEPT
 $CASE1
        KCHOUT=0, KPRNT=006, KPTINV(1)=006, KRUN=1,
        TMIN=-460., TMAX=4000., WTMAX=10000.,
        DTIME=10., START=0., TIMEMX=1200., MAXSSI=4,
        MAXSLP=3,
        MINSSI=3 $
 $PROP1
        CPCO2=.197, CPDIL=.24, VISGAS=.045, WTMTC=16.,CPTC=1.,
        XKGAS=.0147,WTMDIL=28.,WTMCON=18.,CPCONV=.44,
        CPCONL=1., CP(1)=1., RHO(1)=60.1, VISC(1)=0.704,
        WTM(1)=18., XK(1)=.394,CPOXY=.22,
        CP(2)=1. , RHO(2)=62.4,  VISC(2)=3.90,
        WTM(2)=18., XK(2)=.325    $
ID**    1      SOURCE OF CABIN AIR TO SUBSYSTEM
  AS    1      49                2
  RY    01   1 82,288            TOTAL FLOW                             (LB/HR)
VARY    01   4 14.7              PRESSURE                               (PSI)
VARY    01  02 75.               TEMPERATURE                            (F)
```

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VARY   01  06 0,766            WATER VAPOR                    (LB/HR)
VARY   01  07 0,
~~VARY   01  10 18,8             O2                             (LB/HR)~~
VARY   01  11 62,23            N2                             (LB/HR)
VARY   01  12 0,4918           CO2                            (LB/HR)
~~VARY   01  13 ,001~~
ID**    2     SUBSYSTEM BLOWER
KBAS    2     23               1 2                                           8
~~NSTR    2    003~~
VARY    2  91 60,              HEAT ADDED TO AIR STREAM       (WATTS)
ID**    3     ADSORBING SILICA GEL BED
~~KBAS    3     11               8 2                 -12 0   2                 13~~
NSTR    3    211
VARY    3  66 1,
~~VARY    3  67 65,~~
VARY    3  68 0,85             HEAT EXCHANGER EFFECTIVENESS
VARY    3  76 ,05              AVERAGE SS BED LOADING         (LB/LB)
~~VARY    3  79 ,432             COEFFICIENT A~~
VARY    3  80 1062,            COEFFICIENT B
VARY    3  83 1,               FRONTAL AREA                   (SQ FT)
~~VARY    3  84 1,8              LENGTH                         (FT)~~
VARY    3  85 507,             AV,SUPERFICIAL SURFACE AREA    (SQ FT/CU FT)
VARY    3  86 0,4              VOID FRANTION
~~VARY    3  87 ,22              PELLETT SPECIFIC HEAT          (BTU/LB-F)~~
VARY    3  88 45,              PELLET BULK DENSITY            (LB/CU FT)
VARY    3  89 0,01             MASS TRANSFER COEF,            (LB/HR-SQFT-MM HG)
~~VARY    3  90 1,               MASS OF COOLANT ON HX          (LB)~~
VARY    3  91 1,               EXIT ADSORBATE PARTIAL PRESSURE (MM HG)
VARY    3  99 ,05              BED LOADING                    (LB/LB)
~~VARY    3 107 75,              CARRIER GAS TEMPERATURE        (F)~~
VARY    3 115 75,              BED TEMPERATURE                (F)
VARY    3 123 40,              LIQUID OUTLET TEMPERATURE      (F)
~~ID**    4     AIR/AIR REGENERATIVE HEAT EXCHANGER~~
KBAS    4      4              13 2                 -5 2                        14
VARY    4  67  ,97             HEAT EXCHANGER EFFECTIVENESS
~~NSTR    4         10000        1~~
ID**    5     MOLTEN CARBONATE CELL
KBAS    5     54              14 2                       2                     10
~~KARY    5  16          19~~
VARY    5  01 81,03
VARY    5  02 1022,
~~VARY    5  03 14,7~~
VARY    5  04 14,7
VARY    5  05 81,03
~~VARY    5   6 ,01~~
VARY    5  08 0,22
VARY    5  09 29,
~~VARY    5  10 18,8~~
VARY    5  11 62,23
VARY    5  51 80,              TEMPERATURE MODULE SHELLINS/WALL(F)
5 ~~VARY    5  54 70,              AMBIENT GAS TEMPERATURE        (F)~~
VARY    5  55 ,5               UA INSUL,SURFACE TO AMBIENT    (BTU/HR-F)
VARY    5  57 70,              AMBIENT WALL TEMPERATURE       (F)
4 ~~VARY    5  58 ,05~~
VARY    5  60 70,              STRUCTURAL TEMPERATURE
VARY    5  61 0,               THERMAL CONDUCTANCE TO STRUCTURE(BTU/HR-F)
3 ~~VARY    5  64 ,5               INSULATION THERM,CONDUCTANCE   (BUT/HR-F)~~
VARY    5  65 1600,            HEAT DISSIPATED BY ELEC,HEATER (BTU/HR)
VARY    5  67 30,              CELL VOLTAGE                   (VOLTS)
2 ~~VARY    5  69 ,7               POWER EFFICIENCY               (FRACTION)~~
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VARY    5   72 .1             CONVERGENCE TOLERANCE          (PER CENT)
VARY    5   77 75.            CELL THERMAL CAPACITANCE       (BTU/F)
VARY    5   78 1022.          INITIAL CELL TEMPERATURE       (F)
[illegible]*    6      OXYGEN GAS ACCUMULATOR
KBAS    6      30        -5                                              7
NSTR    6     0210
VARY    6   54 75.            AMBIENT GAS TEMPERATURE        (F)
VARY    6   55 2.0            UA TO SURROUNDINGS             (BTU/HR-F)
VARY    6   67 1.0            WEIGHT GAS IN TANK             (LB)
VARY    6   68 75.            TEMP. GAS IN TANK              (F)
VARY    6   69 2.             VOLUME GAS IN TANK             (CU FT)
VARY    6   70 14.7           GAS PRESSURE                   (PSI)
VARY    6   71 1.0            WEIGHT NON-CONDENSABLES        (LB)
VARY    6   76 1.0            WEIGHT OXYGEN                  (LB)
ID**    7      DESORBING SILICA GEL BED
KBAS    7      11        -4 2                 -11 0   1                  2
VARY    7   66 1.
VARY    7   67 65.
VARY    7   68 0.85           HEAT EXCHANGER EFFECTIVENESS
VARY    7   76 0.05           AVERAGE SS BED LOADING         (LB/LB)
VARY    7   79 .432           COEFFICIENT A
VARY    7   80 1062.          COEFFICIENT B
VARY    7   83 1.             FRONTAL AREA                   (SQ FT)
VARY    7   84 1.8            LENGTH                         (FT)
VARY    7   85 507.           SUPERFICIAL SURFACE AREA       (SQ FT/CU FT)
VARY    7   86 0.4            VOID FRACTION
VARY    7   87 .22            PELLET SPECIFIC HEAT           (BTU/LB-F)
VARY    7   88 45.            PELLET BULK DENSITY            (LB/CU FT)
[illegible]RY    7   89 0.01           MASS TRANSFER COEF.            (LB/HR-SQFT-MM HG)
VARY    7   90 1.             MASS OF LIQUID IN HX           (LB)
VARY    7   91 1.             EXIT ADSORBATE PARTIAL PRESSURE (MM HG)
VARY    7   99 .05            BED LOADING                    (LB/LB)
VARY    7  107 75.            CARRIER GAS TEMPERATURE        (F)
VARY    7  115 75.            BED TEMPERATURE                (F)
VARY    7  123 200.           LIQUID OUTLET TEMPERATURE      (F)
NSTR    7      211
ID**    8      SUBSYSTEM BYPASS VALVE
KBAS    8      10        2 2                  2                          3
NSTR    8     0
VARY    8   65 .0001          SPLIT RATIO SYSTEM BYPASS VALVE
ID**    9      CURRENT CONTROLLER
KBAS    9      15                                                        6
NSTR    9     00011
VARY    9   65 .35            SET POINT                      (MM HG)
VARY    9   66 .40            CONTROLLED VARIABLE(CO2 PP OUT) (MM HG)
VARY    9   73 .1             TIME CONSTANT MAIN SENSOR      (SECONDS)
VARY    9   74 1.             GAIN FOR MAIN ERROR SIGNAL
VARY    9   75 .01            DEADBAND                       (MM HG)
VARY    9   76 .69            PROPORTIONAL BAND              (MM HG)
VARY    9   77 0.1            MAXIMUM SPEED FCE              (1/SEC)
VARY    9   68 30.            CURRENT SETTING                (AMPS)
VARY    9   87 25.            CONSTANT B
VARY    9   88 14.3           CONSTANT A
VARY    9   91 0.5            POSITION OF FINAL CONTRL.ELEMENT
[illegible]**   10     TEMPERATURE CONTROLLER
KBAS   10      15                                                        9
NSTR   10     00011
VARY   10   65 1022.          SET POINT                      (F)
VARY   10   66 1030.          CONTROLLED VARIABLE(TCELL)     (F)
VARY   10   68 0.5            BYPASS VALVE SPLIT RATIO
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VARY  10  73 ,1             TIME CONSTANT MAIN SENSOR       (SECONDS)
VARY  10  74 1,             GAIN FOR MAIN ERROR SIGNAL
VARY  10  75 1,             DEADBAND                        (F)
VARY  10  76 150,           PROPORTIONAL BAND
VARY  10  77 0,1            MAXIMUM SPEED FCE               (1/SEC)
VARY  10  87 0,             CONSTANT B
VARY  10  88 1,0            CONSTANT A
VARY  10  91 0,5            POSITION FCE
ID**  11     SOURCE OF HOT FLUID
KBAS  11     49              0   1
VARY  11  01 100,           FLOW                            (LB/HR)
VARY  11  02 200,           TEMPERATURE                     (F)
VARY  11  04 14,7           PRESSURE                        (LB/SQ IN)
ID**  12     SOURCE OF COLD FLUID
KBAS  12     49              0   2
VARY  12  01 100,           FLOW                            (LB/HR)
VARY  12  02 38,            TEMPERATURE                     (F)
VARY  12  04 14,7           PRESSURE                        (LB/SQ IN)
ID**  13     HX BYPASS VALVE
KBAS  13     10             3 2                     2                   4
NSTR  13    0
VARY  13  65 ,01            HX BYPASS RATIO
ID**  14     HX/BYPASS MIXING
KBAS  14      6             4 2                 13 2                    5
NSTR  14    0
PLOT       5  02  0,        1500,     CELL TEMPERATURE(F)
PLOT       5  12  0,        1,        CO2 LEAVING CELL(LB/HR)
PLOT       5  67  0,        40,       CELL CURRENT(AMPS)
PLOT       9  91  0,        1,        CURRENT CONTROLLER FCE POSITION
PLOT      10  91  0,        1,        TEMPERATURE CONTROLLER FCE POSITION
PLOT      13  65  0,        1,        HX BYPASS VALVE SPLIT RATIO
PLOT      14  06  0,        1,        H2O ENTERING CELL(LB/HR)
PLOT      14  12  0,        1,        CO2 ENTERING CELL(LB/HR)
PLOT      05  29  0,        1,        OXYGEN GENERATED(LB/HR)
ENDC
ENDR
*
```

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*INSERT,GPOLY1,24
C     ****************MECHANICAL FREEZEOUT***********************************
      IF(N .NE. 8) GO TO 14
      HG70=HG(70.)
      V96=VV(9,6)
      IF(NPASS .EQ. 0) V96=A(6)+.1
      R(66)=A(1)*CPA*(70.-A(2))+(V96-A(6))*HG70
   15 R(65)=A(2)+R(66)/(A(1)*CPA)
      A(2)=R(65)
   14 CONTINUE
      IF( NPASS .NE. 60  )  GO TO 17
      IF( N  .NE. 2) GO TO 17
      M=1902
      CALL SK(M,6,2)
      M=-1101
      CALL SK(M,6,5)
      M=602
      CALL SK(M,14,2)
      M=600000
      CALL SK(M,18,8)
      M=1400000
      CALL SK(M,6,8)
      M=210010002
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      CALL SK(M,6,9)
      M=502
      CALL SK(M,10,2)
      M=-1601
      CALL SK(M,10,5)
      M=700000
      CALL SK(M,10,8)
      M=210010001
      CALL SK(M,10,9)
      M=-1002
      CALL SK(M,5,5)
      M=1000000
      CALL SK(M,5,8)
      DO 16 LL=1,14
      VR5LL=VV(6,LL)
      VR10LL=VV(10,LL)
      CALL SV(VR5LL,10,LL)
      CALL SV(VR10LL,6,LL)
   16 CONTINUE
   17 CONTINUE
*I GPOLY2,21
      IF(N,NE,20) GO TO 20
      VV12=VV(1,2)
      VV112=VV(1,12)
      VV16=VV(1,6)
      VV192=VV(19,2)
      CALL SV(VV112,20,20)
      CALL SV(VV12,20,21)
      CALL SV(VV16,20,22)
      CALL SV(VV192,20,23)
   20 CONTINUE
TAPE
BASIC           1      -1       15       10     YEA        NAY
CASE          MECHANICAL FREEZOUT SYSTEM PERFORMANCE ANALYSIS
 $CASE1
  KCHOUT=0, KPRNT=6, KPTINV(1)=15,MAXSLP=7, MINSSI=2, KRUN=1, DTIME=30,,
  TIMEMX=3600,,MAXSSI=5, TMAX=250,,TMIN=-450,,WTMAX=1,E4 $
 $PROP1
 CP(1)=,239,RHO(1)=,16   ,VISC(1)= ,036 ,WTM(1)=28,0    ,XK(1)=,007     ,
 CP(2)=1,,RHO(2)=62,4    ,VISC(2)= 3,6  ,WTM(2)=18,0    ,XK(2)=,325     ,
 CP(3)=,175,RHO(3)=,25   ,VISC(3)= ,036 ,WTM(3)=44,0    ,XK(3)=,007     ,
  CPCONL=1,, CPCONV=0,44, CPCO2=0,2, CPDIL=0,25, CPOXY=0,22, CPTC=0,2,
  GAMGAS=1,4, VISGAS=0,44, WTMCON=18,, WTMDIL=28,, WTMTC=20,,
  CPCO2 = ,178,
  XKGAS=0,146 $
ID**    1    1 DUMMY COMPONENT WHICH DEFINES THE INFLUENT TO THE MECHANICAL FREEZO
ID**    1    2 SYSTEM , THE INLET CONDITIONS OF THE H2O CONDENSER,
KBAS    1     49                2
NSTR    1                            DUMMY COMPONENT PASSES A,B-ARRAYS TO R-ARRAY
VARY    1    1   111,6          TOTAL FLOW INTO THE MECH FREEZONT SYS          (LB/HR)
VARY    1    2    70,0          FLUID TEMPERATURE
VARY    1    3    14,7          UPSTREAM DUCT OUTLET PRESSURE                    (PSI)
VARY    1    4    14,7          COMPONENT OUTLET PRESSURE                        (PSI)
VARY    1    5   110,427        NON-CONDENSABLE FLOW                           (LB/HR)
VARY    1    6     1,17         CONDENSABLE VAPOR FLOW                         (LB/HR)
VARY    1    7    0,0           CONDENSABLE ENTRAINED LIQUID FLOW              (LB/HR)
VARY    1    8     ,24          NON-CONDENSABLE SPECIFIC HEAT               (BTU/LB-F)
VARY    1    9    28,97         NON-CONDENSABLE MOLECULAR WEIGHT            (LBS/MOLB)
VARY    1   10    29,35         OXYGEN FLOW                                    (LB/HR)
VARY    1   11    80,41         DILUENT (N2) FLOW                              (LB/HR)
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VARY   1  12     .667      CO2 FLOW                                            (LB/HR)
ID**   2      H2O CONDENSER,ASSUME 100 PER CENT WATER SEPARATION GAS-LIQUID HX
KBAS   2       4            1 2                     -12 0   2              3
   R   2      211000100              PRIMARY OUTLET TEMP CRITERIA FOR SIZING HX
VARY   2  66    93.5       OVERALL UA                                     (BTU/HR-F)
VARY   2  74     3.0       NTU (MAX                                            (ND)
VARY   2  75    45.0       DESIGN OUTLET TEMPERATURE FOR PRIMARY SIDE      (DEG-F)
VARY   2  76     3.0       TOLERANCE FOR PRIMARY SIDE DESIGN OUTLET TEMP,DEG-F.
ID**  12      DUMMY COMPONENT PROVIDING COOLANT/SEC FLOW TO H2O CONDENSER ,COMP,
KBAS  12       49           0  2
VARY  12   1  270.0        COOLANT FLOWRATE                                    (LB/HR)
VARY  12   2   38.0        COOLANT TEMPERATURE                                 (DEG-F)
VARY  12   3   15.0        COOLANT PRESSURE                                    (PSI)
VARY  12   4   15.0        COOLANT PRESSURE                                    (PSI)
ID**  19      DUMMY COMPONENT PROVIDING THE TRICKLE FLOW TO CO2 SUBLIMATOR
ID**   3      SILICA GEL BED FOR H2O ADSORPTION,INTEGRAL HEAT EXCHANGER
KBAS   3       11          2 2                      -13 0   2              4
NSTR   3      202                    H2O ADSORPTION WITH INTEGRAL HX EFFECT,-.88
VARY   3  66    1.          EFFECTIVE HEAT EXCHANGER AREA               NFT**2E
VARY   3  67      65.
VARY   3  68     0.85      HEAT EXCHANGER EFFECTIVENESS
VARY   3  76     0.055     AVERAGE STEADY STATE BED LOADING                    (LB/HR)
VARY   3  79      .432     COEFICIENT FOR H2O ADSORPTION                       (ND)
VARY   3  80 1062.0        COEFICIENT FOR H2O ADSORPTION                       (ND)
VARY   3  83   1.0           ADSORPTION FRONTAL AREA (FT**2)
VARY   3  84   1.8           ADSORPTION BED LENGTH (FT)
VARY   3  85 507.            SUPERFICIAL SURFACE AREA PER VOLUME OF BED 1/FT
VARY   3  86 0.40            VOID FRACTION OF THE PACKED BED
  RY   3  87 .22             SPECIFIC HEAT OF BED MATERIAL BTU/LB-F
  RY   3  88 45.             BULK DENSITY OF BED MATERIAL LB/FT**3
VARY   3  89    .01          MASS TRANSFER COEFFICIENT BETWEEN GAS AND ADSORBEN
VARY   3  90     4.0         MASS OF COOLANT IN HX
VARY   3  91   1.0 E-10  98 EXIT ADSORBATE GAS PRESSURE                       MAHG
VARY   3  99   1.0 E-19 106 BED LOADING (LB ADSORBATE/LB BED)
VARY   3 107  45.0      114 CARRIER GAS OUTLET TEMP                           DEG-F
VARY   3 115  40.0      122 ADSORBENT BED TEMP                                DEG-F
VARY   3 123  40.0      130 LIQUID COOLANT OUTLET TEMP                        DEG-F
ID**  13      DUMMY COMPONENT PROVIDING COOLANT/SEC FLOW TO SILICA GEL BED ,ADSOR
KBAS  13       49           0  2
VARY  13   1  270.0        COOLANT FLOWRATE                                    (LB/HR)
VARY  13   2   38.0        COOLANT TEMPERATURE                                 (DEG-F)
VARY  13   3   15.0        UPSTREAM DUCT OUTLET PRESSURE                       (PSI)
VARY  13   4   15.0        COMPONENT OUTLET PRESSURE                           (PSI)
ID**   4      DUMMY COMPONENT SIMULATING A HEATER THAT IS OFF,DATA PASSES UNCHANG
KBAS   4       49          3 2                                             5
NSTR   4                             ALTCOM PASSES DATA UNCHANGED
ID**   5      REGENERATIVE HEAT EXCHANGER GAS-GAS COUNTERFLOW WITH EFFICIENCY-.95
KBAS   5       4          4 2  3                    -6 2                   6
NSTR   5      211010000              REGEN HX UA GIVEN PRI OUTLET TEMP SIZNG CRITER
VARY   5  66  210.0        OVERALL UA                                 (BTU/HR-DEG-F)
VARY   5  74     8.5       NTU(MAX)                                            (ND)
VARY   5  75 -190.0        DESIGN OUTLET TEMP FOR PRIMARY SIDE                 (DEG-F)
ID**   6      CO2 PERCIPITATOR A GAS-GAS HX WITH PERCIPITATING CO2, NSTR(9)-1
KBAS   6       4          5 2  3                    -16 1   1              7
  TR   6      210010001     1        PRECIP HX UA GIVEN PRT OUT TMP SIZING CRITERIA
VARY   6   1  109.92       TOTAL FLOW                                          (LB/HR)
VARY   6   2 -217.4        TEMPERATURE                                         (DEG-F)
VARY   6   3   13.7        UPSTREAM DUCT OUTLET PRESSURE                       (PSI)
VARY   6   4   13.7        COMPONENT OUTLET PRESSURE                           (PSI)
VARY   6   5  109.89       NON-CONDENSABLE FLOW                                (LB/HR)
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VARY    6   8      ,242        NON CONDENSABLE SPECIFIC HEAT                  (BTU/LB=F)
VARY    6   9    28,97         NON CONDENSABLE MOLECULAR WEIGHT              (LB/MOLE)
~~VARY    6  10    29,35         OXYGEN FLOW                                      (LB/HR)~~
   Y    6  11    80,41         DILUENT FLOW                                     (LB/HR)
VARY    6  12    ,12505        DILUENT FLOW                                     (LB/HR)
~~VARY    6  66    35,0          OVERALL UA                                (BTU/HR=DEG=F)~~
VARY    6  74     3,0          NTU(MAX)                                            (ND)
ID**   16      DUMMY COMPONENT PROVIDING THE REFRIGERATION FLOW FOR CO2 PRECIPITAT
~~KBAS   16      49                 1  1~~
VARY   16   1    45,0          FLOWRATE                                         (LB/HR)
VARY   16   2  =280,           TEMPERATURE                                     (DEG=F)
~~VARY   16   3    20,           UPSTREAM DUCT OUTLET PRESS                        (PSI)~~
VARY   16   4    20,           PRESSURE COMPONEN OUTLET                          (PSI)
VARY   16   5    45,0          NON=CONDENSABLE FLOW                             (LB/HR)
~~VARY   16   8      ,239        SPECIFIC HEAT                                  (BTU/LB=F)~~
VARY   16   9    28,0          MOLECULAR WEIGHT                              (LBS/MOLE)
ID**    7      FAN SIMULATED ONLY TO AN EXTENT OF HEAT ADDITION TO THE SYSTEM
KBAS    7      23            =5 2  3                                         8
NSTR    7      030                   FAN,ADD HEAT SPECIFIED NO FAN PERFORMANCE CALC
VARY    7  91  100,0           HEAT WHICH IS ADDED TO GAS STREAM                (WATTS)
~~VARY    7  92     1,0          THERMAL CAPACITANCE OF FAN ASSY              (BTU/DEG=F)~~
VARY    7  93    30,0          TEMP OF FAN ASSY, END OF PREVIOS TIME STEP   (DEG=F)
ID**    8      HEATER ,THE REQUIRED POWER INPUT WILL BE COMPUTED BY GPOLY LOGIC
~~KBAS    8      49             7 2  3                                          9~~
NSTR    8      1                     HEATER CHANGES THE TEMPERATURE OF THE FLUID,
ID**    9      DESORB,SILICA GEL BEDS DESORBED BY THE WARM AIR FLOWING OUT OF HEAT
~~KBAS    9      11             8 2  3                                         20~~
NSTR    9     200                    SILICA GEL BED DESORB CYCLE,
  RY    9  66   1,               EFFECTIVE HEAT EXCHANGER AREA             NFT**2E
~~  RY    9  67      65,~~
VARY    9  68      0,85        HEAT EXCHANGER EFFECTIVENESS
VARY    9  76      ,055        AVERAGE SS LOADING FOR H2O REMOVAL BEDS   (BTU/HR=F)
~~VARY    9  79       ,42        THERMAL COEFFICIENT FOR H2O CONDENSATION~~
VARY    9  80 1062,0           THERMAL COEFFICIENT FOR H2O CONDENSATION
VARY    9  83   1,0              ADSORPTION FRONTAL AREA (FT**2)
~~VARY    9  84   1,8              ADSORPTION BED LENGTH (FT)~~
VARY    9  85 507,               SUPERFICIAL SURFACE AREA PER VOLUME OF BED 1/FT
VARY    9  86 0,40               VOID FRACTION OF THE PACKED BED
~~VARY    9  87 ,22                SPECIFIC HEAT OF BED MATERIAL BTU/LB=6~~
VARY    9  88 45,                BULK DENSITY OF BED MATERIAL LB/FT**3
VARY    9  89    ,01             MASS TRANSFER COEFFICIENT BETWEEN GAS AND ADSORBEN
~~VARY    9  90     4,0            MASS OF COOLANT IN HX~~
VARY    9  91    7,5         98 EXIT DESORBATE GAS PRESSURE                   MMHG
VARY    9  99     ,1       106 BED LOADING  (LB  ADSORBATE/LB BED)
~~VARY    9 107   70,0       114 CARRIER GAS OUTLET TEMP                      DEG=F~~
VARY    9 115   70,0       122 ADSORBENT BED TEMP                           DEG=F
VARY    9 123   40,0       130 LIQUID COOLANT OUTLET TEMP                   DEG=F
~~ID**   20      METERED FLOW TO CABIN OUT OF MECH FREEZOUT SYSTEM,~~
KBAS   20      29 12          9 2                                         17
NSTR   20      1                     METER ALL FLOWS
~~ID**   17             FOR H20 COLLECTION OUT OF H20 CONDENSER   FLOSUM~~
KBAS   17      12               0                                         18
KARY   17  16              1
~~KARY   17  17              2      H2O CONDENSOR PROVIDING THE FLOW~~
  **   18      WATER STORAGE TANK SIMULATED BY TANKG SUBROUTINE
KBAS   18      30          17 0  2                                        10
~~NSTR   18      1100                  H20 RESERVOIR~~
VARY   18  54      70,0        AMBIENT GAS TEMPERATURE                         (DEG=F)
VARY   18  55       5,0        THERMAL CONDUCTANCE  INSULATION AND AMBIENT (B/HR=F)
~~VARY   18  57      60,         AMBIENT WALL TEMP                               (DEG=F)~~
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VARY   18  58     6,0       THERMAL RADIATION FA FACTOR INSULATION TO WALL (FT2)
VARY   18  60    60,        STRUCTURE TEMP                                 (DEG-F)
~~VARY   18  61     5,0       CONDUCTANCE BETWEEN TANK AND STRUCTURE        (BTU/HR)~~
[illegible]Y   18  64    15,0       CONDUCTANCE BETWEEN OUTER WALL AND-INSULAT (B/HR-F)
VARY   18  67      ,5       TOTAL FLUID WEIGHT IN TANK                       (LBS)
~~VARY   18  68    70,0       FLUID TEMP, IN TANK                            (DEG-F)~~
VARY   18  69      ,016     FLUID VOLUME IN TANK                           (FT**3)
VARY   18  70    14,7       FLUID PRESSURE IN TANK                         (PSI)
~~VARY   18  90     2,5       THERMAL CAPACITANCE OF TANK SHELL              (B/LB-F)~~
VARY   18  92     7,0       MAX ALLOWABLE TEMP CHANGE IN ONE ITERATION  (DEG-F)
ID**   11       DUMMY COMPONENT PROVIDING HEATING FLOW TO THE SUBLIMATOR
~~KBAS   11       49          1   1~~
VARY   11   1    45,        TOTAL FLOW OF WARM N2                        (LB/HR)
VARY   11   2  -100,        TEMPERATURE OF N2                            (F)
~~VARY   11   3    20,        PRESSURE                                     (PSI)~~
VARY   11   4    20,        PRESSURE                                     (PSI)
VARY   11   5    45,        NON-CONDENSABLE FLOW                         (LB/HR)
~~VARY   11   8    ,239       SPECIFIC HEAT                                (BTU/LB-F)~~
VARY   11   9   28,         MOLECULAR WEIGHT                             (LBS/MOLE)
ID**   10       CO2 PRECIPITATOR/SUBLIMATOR  A CYCLIC HX
~~KBAS   10        4            19 2   3                  -11 1   1          14~~
NSTR   10      210010002      1     PRECIP HX UA GIVEN PRT OUT TMP SIZING CRITERIA
VARY   10  66    35,0       OVERALL UA                             (BTU/HR-DEG-F)
~~VARY   10  74     3,0       NTU(MAX)                                         (ND)~~
ID**   14       PUMP FOR CO2 COLLECTION FROM CO2-SUBLIMATION HX TO CO2 RESERVOIR,
KBAS   14       22            10 2   3                                       15
~~NSTR   14       0 2                   CO2 PUMP~~
ID**   15       CO2 RESERVOIR SIMULATED BY TANKG RECEIVES FLOW FROM CO2 PUMP,
[illegible]AS   15       30            14 2   3                                       2
~~[illegible]TR   15      1100                   CO2 RESERVOIR~~
VARY   15  54    70,0       AMBIENT GAS TEMPERATURE                        (DEG-F)
VARY   15  55     5,0       THERMAL CONDUCTANCE  INSULATION AND AMBIENT (B/HR-F)
~~VARY   15  57    60,        AMBIENT WALL TEMP                              (DEG-F)~~
VARY   15  58     6,0       THERMAL RADIATION FA FACTOR INSULATION TO WALL (FT2)
VARY   15  60    60,        STRUCTURE TEMP                                 (DEG-F)
~~VARY   15  61     5,0~~       CONDUCTANCE BETWEEN TANK AND STRUCTURE     (BTU/HR)
VARY   15  67      ,5       TOTAL FLUID WEIGHT IN TANK                       (LBS)
VARY   15  68    70,0       FLUID TEMP, IN TANK                            (DEG-F)
~~VARY   15  69   1,          FLUID VOLUME IN TNK                            (FT**3)~~
VARY   15  70    14,7       FLUID PRESSURE IN TANK                         (PSI)
VARY   15  71    0,5        WEIGHT OF NON-CONDENSABLES                   (LBS)
~~VARY   15  74    ,17        N-C SPECIFIC HEAT~~ IN TNK
VARY   15  75    44,        MOLECULAR WEIGHT IN TNK                      (LBS/MOLE)
VARY   15  78    0,5        WEIGHT OF NON-CONDENSABLES                   (LBS)
~~VARY   15  90     2,5       THERMAL CAPACITANCE OF TANK SHELL              (B/LB-F)~~
VARY   15  92     7,0       MAX ALLOWABLE TEMP CHANGE IN ONE ITERATION  (DEG-F)
KBAS   19       49           2   3
~~VARY   19   1 ,6            TOTAL FLOW~~                                   LB/HR
VARY   19   2   -222,       TEMPERATURE                                  (F)
VARY   19   3     ,5                                                     (PSI)
~~VARY   19   4     ,5                                                     (PSI)~~
VARY   19   5     2,0 E-6                                                (LB/HR)
VARY   19   8        ,23                                                 (BTN/LB-F)
VARY   19   9       28,                                                  (LBS/MOLE)
[illegible]RY   19  11     2,0 E-6                                                (LB/HR)
VARY   19  14 ,6            SUBLIMATE FLOW                               LB/HR
~~PLOT        01  02  0,        100,       TEMPERATURE OF AIR INTO THE SYSTEM DEG-F~~
PLOT         9   2  0,        100,       TEMPERATURE OF AIR OUT OF THE SYSTEM DEG-F
PLOT        01  12  0,        1,0        CO2 FLOW INTO THE SYSTEM   LB/HR
~~PLOT         9  12  0,~~        ,5         CO2 IN PROCESS GAS LEAVING LB/HR
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PLOT      14  12  0.          2.0        CO2 TO ACCUMULATOR LB/HR
PLOT      01  06  0.          1.0        WATER VAPOR FLOW INTO THE SYSTEM L3/HR
PLOT       9   6  0.          1.         WATER VAPOR FLOW OUT  THE SYSTEM L3/HR
PLOT       5   2  -200.       0.         TEMP, OF PROCESS GAS ENTERING PRECIP,DEG F
PLOT       6   2  -220.       0.         GAS TEMP OUT OF PRECIP/SUBLIM DEGF
PLOT      10   2  -220.       0.         GAS TEMP OUT OF SUBLIM/PRECIP DEGF
ENDC
ENDR
*
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*INSERT,GPOLY1,24
C      ***************MEMBRANE DIFFUSION*************************************
       IF(N  ,NE, 10) GO TO 83
          B(1)=6,5*A(1)
   83 CONTINUE
       IF( N ,NE, 2 ) GO TO 99
       A(3)=A(3)*2,
       A(4)=A(3)
       A(2)=175,
   99 CONTINUE
*INSERT,GPOLY2,21
       IF(N ,NE, 5)  GO TO 5
       IF(NPASS ,NE, 30) GO TO 15
       CALL SV(2,62 ,1 ,12)
       CALL SV(187,31,1,1)
       CALL SV(185,27,1,5)
   15 CONTINUE
       R(73)=VV(1,6)
       R(75)=VV(1,12)
       R(76)=VV(1,2)
    5 CONTINUE
       IF(N ,NE, 4) GO TO 10
       R(13)=14,7*A(12)*WTMA/(44,0*A(1)) *51,73
       R(14)=14,7*R(12)*WTMA/(44,0*A(1)) *51,73
   10 CONTINUE
TAPE
BASIC          1      26      13      8    YEA      NAY
CASE 1      MEMBRANE MODULE PERFORMANCE ANALYSIS
 $CASE1
  KCHOUT=0, KPRNT=6, KPTINV(1)=10,MAXSLP=4, MINSSI=2, KRUN=1, DTIME=30,,
  TIMEMX=1800,,MAXSSI=3, TMAX=200,,TMIN=-450,,WTMAX=1,E4 $
 $PROP1
 CP(1)=,239,RHO(1)=,16  ,VISC(1)= ,036 ,WTM(1)=28,0   ,XK(1)=,007    ,
 CP(2)=1,,RHO(2)=62,4   ,VISC(2)= 3,6  ,WTM(2)=18,0   ,XK(2)=,325    ,
 CP(3)=,175,RHO(3)=,25  ,VISC(3)= ,036 ,WTM(3)=44,0   ,XK(3)=,007    ,
  CPCONL=1,, CPCONV=0,44, CPCO2=0,2, CPDIL=0,25, CPOXY=0,22, CPTC=0,2,
  GAMGAS=1,4, VISGAS=0,44, WTMCON=18,, WTMDIL=28,, WTMTC=20,,
  CPCO2 = ,178,      WTMCON=18, ,
  XKGAS=0,146 $
ID**   1   1 DUMMY COMPONENT DEFINING THE INLET CONDITIONS TO THE CO2 REMOVAL
ID**   1   2 SYSTEM USING MEMBRANE MODULE
KBAS   1     49         2
NSTR   1                          DUMMY COMPONENT PASSES A,B-ARRAYS TO R-ARRAY
VARY   1   2   70,0          FLUID TEMPERATURE
VARY   1   1  184,64         TOTAL FLOW INTMEMBRANE DIFFUSIONCONCEPT          (LB/HR)
VARY   1   3   14,7          UPSTREAM DUCT OUTLET PRESSURE                    (PSI)
VARY   1   4   14,7          COMPONENT OUTLET PRESSURE                        (PSI)
VARY   1   5  182,60         NON-CONDENSABLE FLOW                             (LB/HR)
VARY   1   6   2,041         CONDENSABLE VAPOR FLOW                           (LB/HR)
VARY   1   7   0,0           CONDENSABLE ENTRAINED LIQUID FLOW                (LB/HR)
VARY   1   8      ,24        NON-CONDENSABLE SPECIFIC HEAT                 (BTU/LB-F)
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VARY    1   9   28.97        NON-CONDENSABLE MOLECULAR WEIGHT              (LBS/MOLE)
VARY    1  10   48.96        OXYGEN FLOW                                      (LB/HR)
~~VARY    1  11  132.54        DILUENT (N2) FLOW                                (LB/HR)~~
  RY    1  12    1.10        CO2 FLOW                                         (LB/HR)
 D**    2   1 SYSTEM COMPRESSOR USED FOR PRESSURIZING THE INLET FLOW TO ESTABLISH
ID**    2   2 A HIGHER PRESSURE DIFFERENTIAL
KBAS    2     23             1 2                                          3
NSTR    2    0030                   COMPRESSOR REQUIRING Q VS. DELP TABLE
~~ID**    3     CONDENSING HEAT EXCHANGER PROVIDED FOR HUMIDITY CONTROL~~
KBAS    3      4             2 2                  -23 0   2               4
NSTR    3    210001100        1     HX USINX TRANSIEN NO-SIZING GAS LIQUID
VARY    3  66   75.          OVERALL UA                                  (BTU/HR-F)
VARY    3  67     .90        HX EFFECTIVENESS                            (ND)
VARY    3  74    5.0         NTU(MAX)                                    (ND)
~~VARY    3  75      80.       DESIGN  OUTLET TEMP PRI SIDE                (F)~~
VARY    3  76       5.       DESIGN  OUTLET TEMP TOLERANCE               (F)
ID**   23     DUMMY COMPONENT PROVIDING COOLANT FLOW TO THE HEAT EXCHANGER
KBAS   23      49             0  2
NSTR   23     0                     DO NO MODIFY R-ARRAY
VARY   23   1       60.      FLOW.                                       (LB/HR)
~~VARY   23   2       38.      TEMP.                                       (F)~~
VARY   23   3       15.      PRESS.                                      (PSI)
VARY   23   4       15.      PRESS.                                      (PSI)
ID**    4     MEMBRANE MODULE FOR REMOVAL OF CO2 BY SELECTIVE DIFFUSION
KBAS    4      55            3 2                  -13 2                   5
NSTR    4                           NSTR NOT REQRD
~~KARY    4  16          940   NUMBER OF MEMBRANES IN THE MODULE~~
VARY    4  54     70.        AMBIENT GAS TEMP.                           (F)
VARY    4  55      1.3       THERMAL CONDUCTANCE BTWN SURFACE + AMBENT (BTU/HR-F)
~~  RY    4  57     60.        AMBIENT WALL TEMP                           (F)~~
VARY    4  58      6.        FA FACTOR FOR RADIATION                     (FT**2)
VARY    4  60     60.        STRUCTURE TEMP                              (F)
~~VARY    4  61     12.        CONDUCTANCE BETWEEN MODULE AND STRUCTURE    (BTU/HR-F)~~
VARY    4  65      2.0       MEMBRANE AREA                               (FT**2)
VARY    4  66    .005        THICKNESS                                   (IN)
~~VARY    4  69    1.2 E-5     CO2 PERMEABILITY~~
VARY    4  91       1.71     INTERNAL THERMAL CONDUCTANCE , PRI.         (BUT/HR-F)
VARY    4  92       1.71     INTERNAL THERMAL CONDUCTANCE , SEC.         (BTU/HR-F)
~~VARY    4  93     10.8       EFFECTIVE THERMAL CONDUCTIVITY THROUGH MEMBRANES 4~~
VARY    4 103      2.0       MODULE LENGTH                               (FT)
VARY    4 104       .1       FRONTAL AREA  PRIMARY SIDE                  (FT**2)
VARY    4 105       .1       FRONTAL AREA  SECONDARY SIDE                (FT**2)
VARY    4 106     12.0       THERMAL CAPACITANCE OF MODULE SHELL         (BTU/F)
VARY    4 107        .95     MULT. FACTOR USED  IN COMPUTIN  STABILITY CRITERIA
~~VARY    4 108      5.        MINIMUM TIME INCREMENT IN TRANSIENT SOLUTION~~
ID**    5     FLOW METER EVALUATING THE AIR FLOW FROM THE CO2 REMOVAL SYSTEM
KBAS    5     29 12          4 2                                          6
~~NSTR    5     1                     METER ALL CONSTITUENTS (FLOWMETER)~~
VARY    5  65    0.          REFERENCE TEMPERATURE FOR ENTHALPY          (F)
ID**    6     CONDENSING HX FOR SEPARATION OF CO2 FROM H2O VAPOR
~~KBAS    6      4            -4 2                  -26 0   2               7~~
NSTR    6     210001100       1
VARY    6  66  460.          OVERALL UA                                  (BTU/HR-F)
VARY    6  67      .90       HX EFFETIVENESS                             (ND)
  RY    6  74     5.         NTU(MAX)                                    (ND)
  RY    6  75 40.            DESIGN OUTLET TEMP  PRI SIDE                (F)
~~VARY    6  76 3.             TOLERANCE FOR DESIGN TEMP                   (F)~~
ID**   26     DUMMY COMPONENT PROVIDING COOLANT FLOW TO THE CONDENSOR
KBAS   26      49             0   2
NSTR   26     0                     DO NOT MODIFY R-ARRY
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VARY  26   1    270.          FLOW                                              (FLOW)
VARY  26   2     35.          TEMP.                                             (TEMP)
~~VARY  26   3     15.          PRESS.                                            (PSI)~~
VARY  26   4     15.          PRESS.                                            (PSI)
ID**   7      CO2 PUMP USED TO FORCE CO2 INTO THE ACCUMULATOR
~~KBAS   7      23            6 2                                                  8~~
NSTR   7     0030                        ADD HEAT SPECIFIED IN R(91) ONLY
VARY   7  91    .01           HEAT ADDED TO GAS STREAM                          WATTS
~~ID**   8      CO2 ACCUMULATOR~~
KBAS   8      30              7 2                                                  9
NSTR   8     1100
~~VARY   8  54    70.           AMBIENT GAS TEMPERATURE                           (F)~~
VARY   8  55     5.           THERMAL CONDUCTANCE BETWEEN AMBIENT TANK          (BTN/HR-F)
VARY   8  57    60.           AMBIENT WALL TEMP                                 (F)
~~VARY   8  58     6.           RADIATION FA FACTOR SKIN TO WALL                  (FT**2)~~
VARY   8  60    60.           STRUCTURE TEMPERATURE                             (F)
VARY   8  61    12.           CONDUCTANCE BETWEEN TNK WALL AND STRUCTUR         (BTU/HR-F)
~~VARY   8  67      .5          TOTAL FLUID WEIGHT IN TNK                         (LBS)~~
VARY   8  68    70.           FLUID TEMPERATURE IN TNK                          (F)
VARY   8  69     1.           FLUID VOLUME IN TANK.                             (FT**3)
~~VARY   8  70    14.7          FLUID PRESS IN TNK                                (PSI)~~
VARY   8  71     0.5          WEIGHT OF NON-CONDENSABLE IN TNK                  (LBS)
VARY   8  74      .17         NON-CONDENSABLE SPECIFIC HEAT IN TNK.             (BTU/LB-F)
~~VARY   8  75    44.           NON-CONDENSABLE MOLECULAR WEIGHT IN TNK.          (LB)~~
VARY   8  78     0.5          WEIGHT OF NON-CONDENSABLE IN TNK                  (LBS)
ID**   9      H2O REMOVAL/SEPARATION ACCOMPLISHED BY THIS UNIT
~~KBAS   9      12              0   2                                              10~~
NSTR   9                                 NSTR CARDS NOT REQRD
KARY   9  16            2
~~KARY   9  17            3~~
KARY   9  18            6
ID**  10      JUNCTION FOR H2O MIX TO SYSTEM FROM THE WATER STORAGE SYSTEM
~~KBAS  10       7              9 0   2                     -14 0   2              11~~
NSTR  10      2                          LIQUID MIX MIXED FLOW PRESS = PRI SOURCE PRESS
ID**  11      H2O ACCUMULATOR STORING WATER THAT IS USED BY STEAM GENERATOR
~~KBAS  11      30            10 0   2                                             12~~
NSTR  11     1100                        GPOLY LOGIC COMPUTES OUTLET FLOW  H2O ACCU.
VARY  11   1 6.5              TOTAL FLOW                                        (LB/HR)
~~VARY  11   2 70.              TEMP                                              (F)~~
VARY  11   3 1.               PRESS                                             (PSI)
VARY  11   4 1.               PRESS                                             (PSI)
~~VARY  11  54     70.          AMBIENT GAS TEMPERATURE                           (F)~~
VARY  11  55      5.          THERMAL CONDUCTANCE INSULATION AND GAS            (BTU/HR-F)
VARY  11  57     60.          AMBIENT WALL TEMPERATURE                          (F)
~~VARY  11  58      6.          THERMAL RADIATION FACTOR FA SKIN TO WALL          (FT**2)~~
VARY  11  60     60.          STRUCTURE TEMPERATURE                             (F)
VARY  11  61     12.          CONDUCTANCE BETWEEN TNK WALL AND STRUCTUR         (BTU/HR-F)
~~VARY  11  67      8.          TOTAL FLUID WEIGHT IN TANK                        (LB)~~
VARY  11  68     70.          FLUID TEMP IN TANK                                (F)
VARY  11  69       .5         FLUID VOLUME IN TANK                              (FT**3)
~~VARY  11  70 1.               PRESS                                             (PSI)~~
VARY  11  73 31.2             WEIGHT OF LIQUID IN TNK                           (LBS)
VARY  11  87 62.4             DENSITY                                           (LB/FTCU)
~~VARY  11  89 18.~~
ID**  12      H2O PUMP FO FORCING WATER TO THE STEAM GENERATOR
KBAS  12      22             11 0   2                                              13
~~NSTR  12      0 2                      ONLY V-ARRY DATA REQRD IS HEAT ADDED TO FLUID~~
VARY  12  85      .1          HEAT ADDED TO FLUID STREAM                        (WATTS)
ID**  13   1 STEAM GENERATOR PROVIDING THE VAPOR FLOW USED AS SWEEP GAS IN THE
~~ID**  13   2 MEMBRANE MODULE FOR CO2 REMOVAL~~
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KBAS  13     27             12 2                                   2
NSTR  13    01                         HEATNG REQRMNTS TO VAPORIZE LIQUID ENTERNG
VARY  13    1 6,5                 TOTAL FLOW OF STEAM                LB/HR
[illegible]RY  13    2 120,                TEMP                               F
VARY  13    3 1,0                 PRESS                              PS1
VARY  13    4 1,0                 PRESS                              PS1
VARY  13    6 6,5                 VAPOR FLOW                         LB/HR
VARY  13    8 ,24                 SPECIFIC HEAT                      BTU/HB-F
VARY  13    9 28,97               MOLECULAR WEIGHT                   LB/MOLE
VARY  13   66      20,            DESIRED DEGREES OF SUPERHEAT       (F)
ID**  14      WATER STORAGE TANK PROVIDING THE MAKEUP WATER FOR MEMBRANE MODULE,
KBAS  14     30               0   2
NSTR  14                               TANK SUPPLYING MAKE-UP WATER
VARY  14    2 70,                 OUTLET TEMP                        F
VARY  14    3 1,0                 OUTLET PRESS                       PS1
VARY  14    4 1,0                 OUTLET PRESS                       PS1
VARY  14   54      70,            AMBIENT GAS TEMP                   (F)
VARY  14   55        0,01         CONDUCTANCE BETWEEN SURFACE AND AMBNT GAS (BTU/HR-F)
VARY  14   57      60,            AMBIENT WALL TEMP                  (F)
VARY  14   58      60,            RADIATION FACTOR FA SURFACE TO WALL    (FT**2)
VARY  14   60      60,            STRUCTURE TEMP                     (F)
VARY  14   61         ,01         CONDUCTANCE KA/X TANK TO STRUCTURE
VARY  14   68 70,                 FLUID TEMP IN TNK                  F
VARY  14   70 1,0                 PRESS, IN TNK                      PSI
VARY  14   91         ,01         THERMAL CONDUCTANCE INTERNAL FLUID TANK   (BTU/HR-F)
VARY  14   92        5,0          MAX ALLOWABLE TEMP CHANGE          (F)
PLOT        1  12   0,            3,0        CO2 FLOW INTO CONCENTRATOR LB/HR
PLOT        4  12   0,            3,0        CO2 FLOW OUT OF THE CONCENTRATOR  LB/HR
PLOT        5  76  40,            100,       TEMPERATURE OF AIR FLOWING IN  DEG-F
[illegible]T        4   2  40,            100,       TEMPERATURE OF AIR FLOWING OUT DEG-F
PLOT        4  13   0,            10,0       PPCO2 OF GAS STREAM FLOWING IN  MMHG
PLOT        4  14   0,            10,0       PPCO2 OF GAS STREAM FLOWING OUT MMHG
PLOT        5  73   0,            3,0        H2O FLOWRATE INTO CO2 CON, SYS  LB/HR
PLOT        4   6   0,            3,0        H2O FLOWRATE OUT OF CO2 CONT, SYS, LB/HR
ENDC
ENDR
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