NASA CR-112098

A TRANSIENT PERFORMANCE METHOD FOR CO_2 REMOVAL WITH REGENERABLE ADSORBENTS

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Prepared Under
Contract No. NAS 1-8559

by

AIRESEARCH MANUFACTURING COMPANY
Los Angeles, California

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National Aeronautics and Space Administration
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FOREWORD

Part I of this report describes a computer program (S9960) which can be used to predict the transient performance of vacuum-desorbed sorbent beds for CO_2 or water removal, and composite beds of two sorbents for simultaneous humidity control and CO_2 removal. The program was written primarily for silica gel and molecular-sieve inorganic sorbents, but can be used for a variety of adsorbent materials.

The initial development of the computer program was started under the Apollo Applications Program, Contract NAS9-3541, NASA Manned Spacecraft Center. Further improvements were made through the application of AiResearch R & D funds, and under Contract NAS1-8559 from the NASA Langley Research Center which also funded the acquisition of additional basic adsorption data.

The content of Part I is as follows: Section 1 presents a general description of the program; Section 2 describes the technical details of the program; Section 3 describes program usage; and Section 4 presents an example of program usage; Subroutine documentation is given in Section 5, together with a complete listing of the program.

Part II of this report describes a computer program (MAIN4B) which can be used to predict performance for multiple-bed CO_2-removal sorbent systems. This program is an expanded version of the composite-sorbent-bed program, S9960, described in Part I.

The primary improvement included in MAIN4B is that the poisoning effect of water coadsorbed by the CO_2-removal bed is taken into account in predicting the CO_2 adsorption performance of the bed. The program also estimates coadsorption of oxygen, nitrogen, and subsequent overboard losses. The system simulation capabilities have been expanded to allow consideration of

- 2-bed vacuum-dump,
- 4-bed H_2O-save/CO_2-dump, and
- 4-bed H_2O-CO_2-save type systems.
- Beds may be thermally conditioned by heat-transport fluid passages within the bed, or by internal electrical heaters.

Although certain features of MAIN4B are completely new, or are considerably different from those incorporated in program S9960, much of the background material presented in Part I is used in the new program. Part II presents only material unique to MAIN4B. The complete documentation of the new program, for those interested in the techniques used in the program, or for those desiring to modify the program set, includes both Part I and Part II.

Nomenclature used in this report is presented at the beginning of each part. The content of Part II is as follows. Section 1 provides a general description of the program; Section 2 technically describes new features of MAIN4B that make it different than S9960; Section 3 describes input data for

FOREWORD (Cont)

program execution; and Section 4 presents two example runs with the program. Two appendixes furnish subprogram documentation (Appendix A) and a complete listing of the program (Appendix B).

Dr. K.C. Hwang of AiResearch, developed the computer programs described in this report, and also authored the report.

Mr. Rex Martin of NASA Langley Research Center was the technical monitor of Contract NAS1-8559 during the development of these computer programs.

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PART I

COMPOSITE BED PROGRAM (S9960)

NOMENCLATURE

FORTRAN	Algebraic	Description
A	$\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g}\right)$	Quantity $\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g}\right)$ appearing in Equation (2-35), (lb-mole)/(hr)(sq ft)(mm Hg)
ADT		Temporary storage for DT, hr
ADT2		Temporary storage for DT, hr
ABED	A	Cross-sectional area of adsorbent bed, sq ft
AGS,ASG	a_{sg}	External surface area of sorbent, sq ft/(cu ft of bed)
AGX,AXG	a_{xg}	Primary heat transfer area between heat exchanger and gas stream, sq ft/cu ft of sorbent bed
ASX,AXS	a_{xs}	Primary heat transfer area between heat exchanger and sorbent, identical to a_{xg}
AVC	a_{vc}	Primary heat transfer area for coolant, sq ft/(cu ft of coolant volume)
AVLD		Average loading at each axial node, (lb-sorbate)/(lb-sorbent)
AVH2OP		Average poisoning rate of molecular sieves by H_2O, (lb-H_2O)/hr
AVMSLD		Average CO_2-loading of all active molecular sieve sorbents, lb-CO_2/(lb-molecular sieves)
AVPH2O		Average outlet P_{H_2O}, mm Hg
AVRCO2		Average CO_2 adsorption or desorption rate, lb-CO_2/hr
AVRH2O		Average H_2O adsorption or desorption rate, lb-H_2O/hr
AVSGLD		Average H_2O-loading of desiccant sorbents, lb-H_2O/(lb-desiccant)
AVX	a_{vx}	Primary heat transfer area for heat exchanger, sq ft plate area/(cu ft of metal)
B		Temporary variable used in simultaneous solution of a system of finite difference equations. See Equations (2-41) and (2-42)

FORTRAN	Algebraic	Description
C	C	Molal density of gas mixture, lb moles/(cu ft)
CPC	C_{pc}	Heat capacity of coolant, Btu/(°F)(lb)
CPG	C_{pg}	Heat capacity of gas mixture, Btu/(°F)(lb)
CPS	C_{ps}	Sorbent specific heat, Btu/(lb)(°F)
CPX	C_{px}	Heat capacity of heat exchanger metal, Btu/(°F)(lb)
CP1, CP2		Coefficients in equation $PC3 \cdot \left(P_{ks_{t+\Delta t}} - X_k P_{t+\Delta t}\right) = CP1 + CP2 \cdot P_{t+\Delta t}$
CR1, CR2, CR3		Coefficients in following equation which is merely another form of Equation (2-28). $CR1 \cdot \frac{W_{k,M,(t+\Delta t)} - W_{k,M,t}}{(\Delta t)} = CR2 \cdot \left(W_{k,(M-1)(t+\Delta t)} - W_{k,M,(t+\Delta t)}\right) + CR3 \cdot \left(W_{k,M,(t+\Delta t)} - W_{k,(M+1),(t+\Delta t)}\right)$
CS1, CS2		Coefficients in equation $T_{s(t+\Delta t)} - T_{s,t} = DS + CS1 \cdot P_{(t+\Delta t)} - CS2 \cdot P_{ks,(t+\Delta t)}$
CYCLE		Cycle time per one adsorption or one desorption half-cycle, hr
C1, C2, C3		Coefficients in equation $C_1 \cdot W_{(t+\Delta t),(M-1)} + C2 \cdot W_{(t+\Delta t),M} + C3 \cdot W_{(t+\Delta t),(M+1)} = D1$
C1P, C2P, C3P		Coefficients in equation $C1P \cdot P_{(t+\Delta t),(N-1)} + C2P \cdot P_{(t+\Delta t),N} + C3P \cdot P_{(t+\Delta t),(N+1)} = D1P$
DH	ΔH	Heat of adsorption at each node Btu/(lb adsorbed)
DIF	D_k	Mass diffusivity of component k through the interior of sorbent, sq ft/hr

FORTRAN	Algebraic	Description
DPCφ2C		Cabin CO_2 partial pressure increase in one time increment, mm Hg
DS		See CSI
DTφ		Time increment of previous computation step, hr
DT	Δt	Time increment, hr
DTMAX		Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
DVS		Size of interior sorbent volume elements, (cu ft)
DVSI		Size of sorbent volume elements at surface and center of spherical pellets, DVSI = 1/2 DVS, (cu ft)
DX		Axial node dimension, ft
DI		See CI
DIP		See CIP
D2		Coefficient in equation $W_{ks_{(t+\Delta t)}} = Q + D2 \cdot P_{(t+\Delta t)}$
D9		DT in single precision, hr
F	F	Factor defined by Equation (2-17), a function of pressure
FR		Molal flow rates of CO_2 and H_2O, during desorption, FR(1,N) is CO_2 rate, FR(2,N) is H_2O rate, lb-mole/hr
	G	Mass flux = $u_g \cdot \rho_g$, lb/(hr)(sq ft void area)
GK	K_g	Mass transfer coefficient between bulk stream and the surface of adsorbent. Surface kinetic rate can be incorporated in this coefficient, lb-moles/(hr)(sq ft)(mm Hg)
GMR	G_t	Total mass flow rate, lb/(hr)
GMW	M_g	Average molecular weight of process gas
HCX,HXC	h_{xc}	Heat transfer coefficient between heat exchanger primary plate and coolant, Btu/(sq ft)(^oF)(hr)

FORTRAN	Algebraic	Description
HGS,HSG	h_{sg}	Heat transfer coefficient between sorbent and gas, based on a_{sg}, Btu/(sq ft)(^{0}F)(hr)
HSX,HXS	h_{xs}	Effective heat transfer coefficient between heat exchanger primary plate and sorbent, Btu/(sq ft)(^{0}F)(hr)
$\dot{M}_{sg}$		Molal rate of mass transfer into bulk gas stream/unit bed volume, lb-moles per (cu ft of bed)(hr); see Equation (2-15)
M_s		Interior node corresponding to the surface of pellet
NBCØUT		Integer control variable, if NBØUT = 2, the outlet manifold pressure is specified as a function of time; NBØUT = 1, the manifold pressure is computed from vacuum duct resistance
NCYCLE		Number of complete adsorption-desorption cycles from beginning of run
NCYCLT		Total number of complete adsorption-desorption cycle calculations desired
NDR4		Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDTCØN		If = 1, internal Δt calculations. If = 2, fixed Δt's in program will be used.
NDXM		Integer denoting total number of molecular sieve nodes
NDXMAC		Integer denoting number of active molecular sieve nodes, i.e., (NDXM-NDXMAX) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NDXI		Integer denoting total number of axial nodes
NØG		Node to which coolant is added
NPR		Number of time steps elapsed since last printout
NPRINT		Integer control variable which determines the frequency of printout occurrence; e.g., if NPRINT = 5, printout occurs after every five time steps
NPSET		Integers which denote the nodes to which tabulated vacuum history is applicable

FORTRAN	Algebraic	Description
NSTART		Integer denoting the cycle from which on bed performance will be printed at frequency specified by NPRINT
NTEMP		Integer control variable; If NTEMP = 0, the energy equations will be ignored and bed temperatures set equal to T268; If NTEMP $\neq$ 0, heat balances will be performed
PA	P	System total pressure during adsorption, mm Hg
PCØ2C		CO_2 partial pressure in cabin, mm Hg
PCØ2I		CO_2 partial pressure at adsorption bed inlet, mm Hg
PC1 PC2 PC3		Coefficients in equation for desorption pressure $\frac{P_{(t+\Delta t),N} - P_{t,N}}{(\Delta t)} = PC1 \cdot \frac{P_{(t+\Delta t),(N-1)} - 2P_{(t+\Delta t),N} + P_{(t+\Delta t),(N+1)}}{(\Delta x)^2} + PC2 \cdot \frac{P_{(t+\Delta t),(N+1)} - P_{(t+\Delta t),(N-1)}}{2(\Delta x)} + PC3 \cdot [p_{ks(t+\Delta t)} - X_k P_{(t+\Delta t)}]$
PH2ØI		Inlet H_2O partial pressure, mm Hg
PK	p_k	$P \cdot X_k$; partial pressure of component k in bulk gas stream, mm Hg
PØUT		10 tabulated desorption outlet pressures at TIMET, mm Hg
PT	P	Total pressure in bulk gas stream, mm Hg
P1 P2 P3		Coefficients in equation $p_{ks(t+\Delta t)} = P1 + P2 \cdot (W_{k,s(t+\Delta t)} - W_{k,s,t}) + P3 \cdot P$
Q		Temporary variable like B. See Equations (2-43) and (2-44)
	r	Radial distance from center of sphere, ft
	r_M	r at interior node M, ft

FORTRAN	Algebraic	Description
	r_s	Average particle radius found from ρ_{sb} and a_{sg}, ft
RCØ2C		Rate of CO_2 generation in cabin, lb CO_2 per hr
RGAS	R	Gas constant, 554 (mm Hg) (cu ft)/(lb-mole) (^{0}R)
RHØC	ρ_c	Coolant density, lb/(cu ft)
RHØG	ρ_g	Gas density, lb/(cu ft)
RHØS	ρ_s	Sorbent density, lb/(cu ft particle)
RHØSB	ρ_{sb}	Sorbent bulk density, lb/(cu ft bed volume)
RHØX	ρ_x	HX core metal density, lb/(cu ft)
RS	r_s	Average particle radius found from ρ_{sb} and a_{sg}, ft
RSI		Radius of spherical surface separating two interior sorbent volume elements, ft
SK	k_s	Effective thermal conductivity of sorbent bed, Btu/(hr) (sq ft) (^{0}F/ft)
SUMPTM		Quantity $\sum_{t = zero}^{t} P_{H_2O,\ outlet} \cdot (\Delta t)$, (mm) (hr)
TC	T_c	Coolant temperature, ^{0}F
TCI		Coolant temperature at time, $t-\Delta t$
TC2		Coolant temperature at time, $t-2\Delta t$
TG	T_g	Gas temperature, ^{0}F
TGI	T_{gi}	Inlet gas temperature for adsorption cycle, ^{0}F

FORTRAN	Algebraic	Description
TI		Maximum temperature change allowable per time increment in selecting Δt, ^{0}F
TIME	t	Time from beginning of each adorption or desorption period, hr
TIMEM		Time above in minutes.
TIMET		10 times at which PØUT are tabulated, hr
TKX	k_x	Thermal conductivity of heat exchanger core metal, Btu/(hr) (sq ft) (^{0}F/ft)
TØTCØ2		Total amount of CO_2 adsorbed since beginning of adsorption period, lb
TØTH2Ø		Total amount of H_2O adsorbed since beginning of adsorption period, lb
TS	T_s	Sorbent temperature, ^{0}F
TS1		Sorbent temperature at time $t-(\Delta t)$, ^{0}F
TS2		Sorbent temperature at time $t-2(\Delta t)$, ^{0}F
TX	T_x	Heat exchanger core metal temperature, ^{0}F
TX1		Heat exchanger core metal temperature at time $t-(\Delta t)$, ^{0}F
TX2		Heat exchanger core metal temperature at time $t-2(\Delta t)$, ^{0}F
T268	T_{268}	Inlet glycol temperature, ^{0}F
UC	u_c	Coolant velocity, ft/hr
UG	u_g	Interstitial gas velocity, i,e., true gas velocity, ft/hr
VMS		Total bulk volume of molecular sieve sorbents, cu ft

FORTRAN	Algebraic	Description
VØIDF	f	Void fraction of bed
VØLCAB		Cabin volume for atmosphere, cu ft; use VOLCAB = 10^{20}, for constant PCO2C
VS		Volume of a single sorbent pellet, cu ft
VSG		Total bulk volume of desiccants, cu ft
W	W_k	Local loading of component k in sorbent, lb sorbate k/lb sorbent
	$W_d(P)$	A function of pressure which represents the capacity of vacuum duct at duct inlet pressure of P mm, lb/hr
WI		Maximum loading change allowable per time increment in selecting Δt, lb/lb
WM	M_k	Molecular weight of component K. K = 1 and 2
WS		Temporary storage variable for W
WTACMS		Total weight of active molecular sieve sorbents, lb
WTMS		Total weight of molecular sieve sorbents, lb
WTSG		Total weight of desiccants, lb
X	X_k	Mole fraction of component k in gas stream k=1 refers to CO_2 in molecular sieve bed gas stream, and K=2 refers to H_2O in desiccant bed gas stream
	x	Distance from molecular sieve bed end, ft
	Y	Any of bed properties, T_s, T_x, W_k, T_c, T_g

Subscripts

b	Bulk
c	Coolant
g	Gas stream

Subscripts

i Inlet

k Component k

M Radial location index for sorbent interior nodes

N Axial location index

s Surface of sorbent

s Sorbent

t At time t

v Volume

x Heat exchanger

Superscripts

* Equilibrium quantity

SECTION I

GENERAL DESCRIPTION

INTRODUCTION

The present computer program package for the Univac 1108 computer, S9960 through S9999, was developed to predict the transient performance of a composite molecular sieve/desiccant bed for CO_2 removal, which may be operated under either adiabatic or thermal swing conditions. The program is limited to cases where sorbents are regenerated by dumping to vacuum.

An attempt was made to solve the actual physical problem as rigorously and generally as was feasible. Thus, transient pressure variations during a desorption cycle are not arbitrarily set, but are calculated from the AiResearch test data (as shown here) for the flow of nitrogen gas under low pressures through a 5/8-in.-ID molecular sieve bed. For program flexibility, most of the physical properties and transfer rate constants are allowed to vary as a function of the bed location. Such a flexibility allows for the use of different heat exchanger configurations and different modes of operation for the molecular sieve bed and the desiccant bed.

The program does not assume any specific heat exchanger configuration for thermal control and is, therefore, applicable to cases where sorbent temperatures are regulated by cooling coils, plate-fin heat exchangers or process gas streams alone, and so forth. However, to implement this general approach, heat transfer coefficients for heat balance calculations are not computed in the program but must be supplied as input data.

The mass-transfer equations are written to permit both intraparticle diffusion and surface resistance. Either process can be made to control by proper choice of the appropriate coefficients in the input.

To minimize the running time of the program, an implicit scheme as proposed by Hwang (Reference 1) was employed for transient mass transfer calculation and a method somewhat similar to the one proposed by DuFort and Frankel (Reference 2) for solving a diffusion equation was used to handle the coupling terms of the energy equations for the transient temperature changes of the metal parts, the sorbent, and the coolant. The program, therefore, permits the use of allowable large time increments for accuracy considerations.

Program S9960 performs adsorption and desorption calculations for a specified number of complete cycles. Programs S9950 and S9951 perform adsorption and desorption calculations, respectively, for one-half cycle only. With all physical properties and operation parameters inputted through two block data subprograms, the programs will compute and print out temperature and bed loading changes as a function of time. Average bed loadings and average rates of adsorption and desorption are also printed.

MATHEMATICAL MODEL

An example of a sorbent bed for CO_2-removal is depicted in Figure 1-1. The unit shows the detail of construction. It is basically a platefin gas-liquid heat exchanger with sorbents packed between the fins in the gas side.

In the present program, bed properties are assumed to vary only in the direction of the process gas flow, and that coolant is either parallel or counter-current but cannot be cross flow to the gas flow. Electric analogs of the heat transfer in the idealized sorbent bed during adsorption and desorption are shown in Figures 1-2 and 1-3. Figures 1-4 and 1-5 show electric analogs for mass transfer processes involved in the bed during the adsorption and desorption periods, respectively. Although a plate-fin heat exchanger is shown in Figure 1-1, the analogs of Figures 1-2 through 1-5 should still be valid for cases where other means of thermal control are used.

The resistances to thermal transfer in Figures 1-2 and 1-3 can be easily estimated from thermal conductivities of materials used. The mass transfer resistances in Figures 1-4 and 1-5, however, must be determined from actual bed performance data.

Although heat and mass transfer processes are shown separately, a coupling does exist between the two. In Figure 1-2 the "I's" represent the rates of heat generation at various nodes due to various rates of sorbate adsorption by these nodes, which are the mass transfer rates across the sorbent surface resistances shown in Figure 1-4. Similarly the "I's" in Figure 1-3 are coupled with the mass transfer rates in Figure 1-5.

PROGRAM CAPABILITIES

Uses

Program S9950 predicts the performance of a single adsorption period. It is used for analyzing a breakthrough curve that is obtained from a known initial bed conditions, such as an adsorption run which is made immediately after a bakeout. By a few trial-and-error runs of this program, the mass transfer coefficient and mass diffusivity for the test system can be found.

Program S9951 predicts the performance of a single vacuum desorption period. It is used to determine mass transport properties of a sorbent-sorbate system if a desorption run started from known initial conditions is available.

Program S9960 is designed to predict the performance of a cyclically regenerated adsorption-desorption system comprising a desiccant and a CO_2 sorbent bed. Although the program is not designed for bed-sizing, no more than three trials are usually required to zero in on a correct design to meet

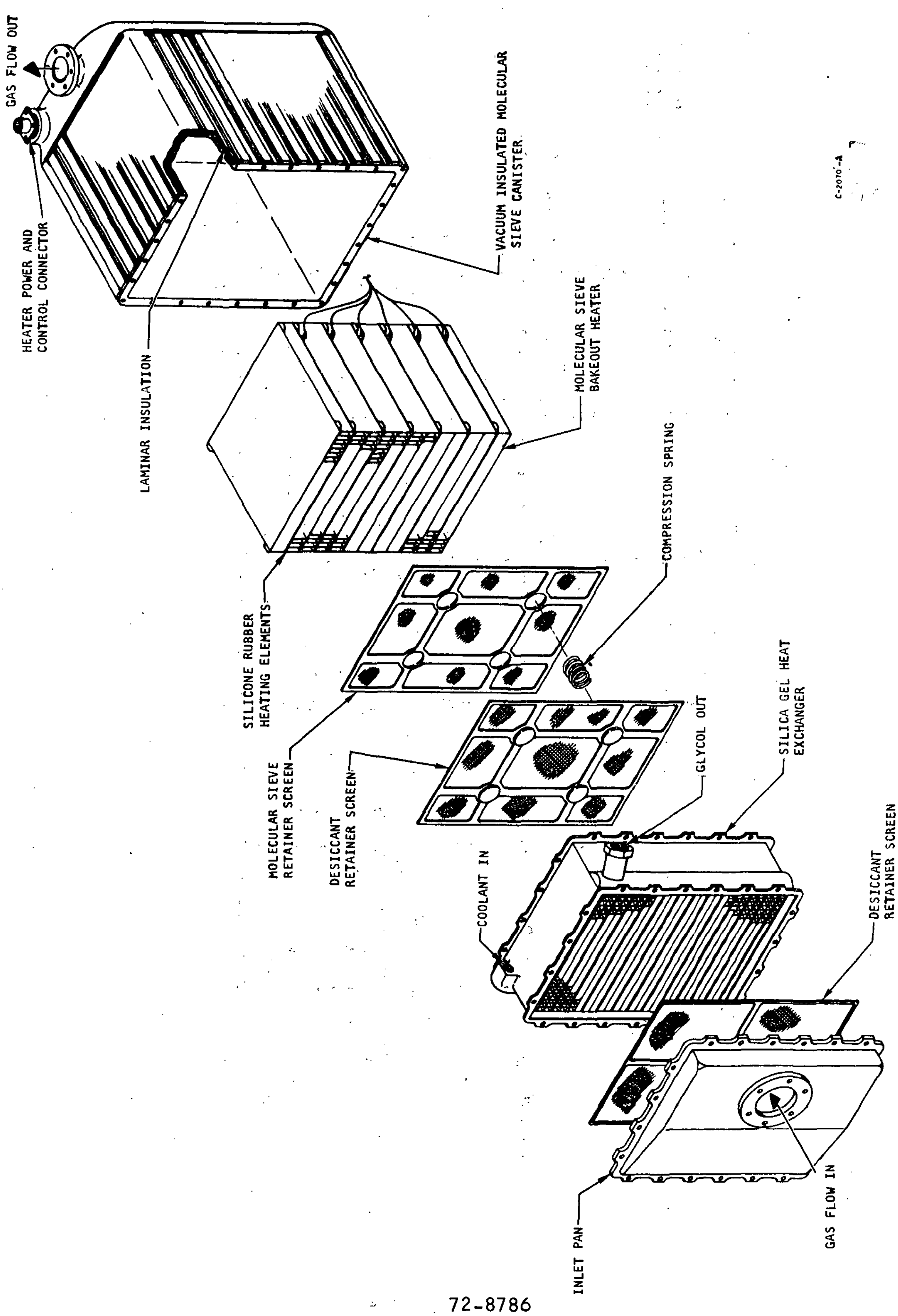

Figure 1-1. Typical Adsorbent Canister

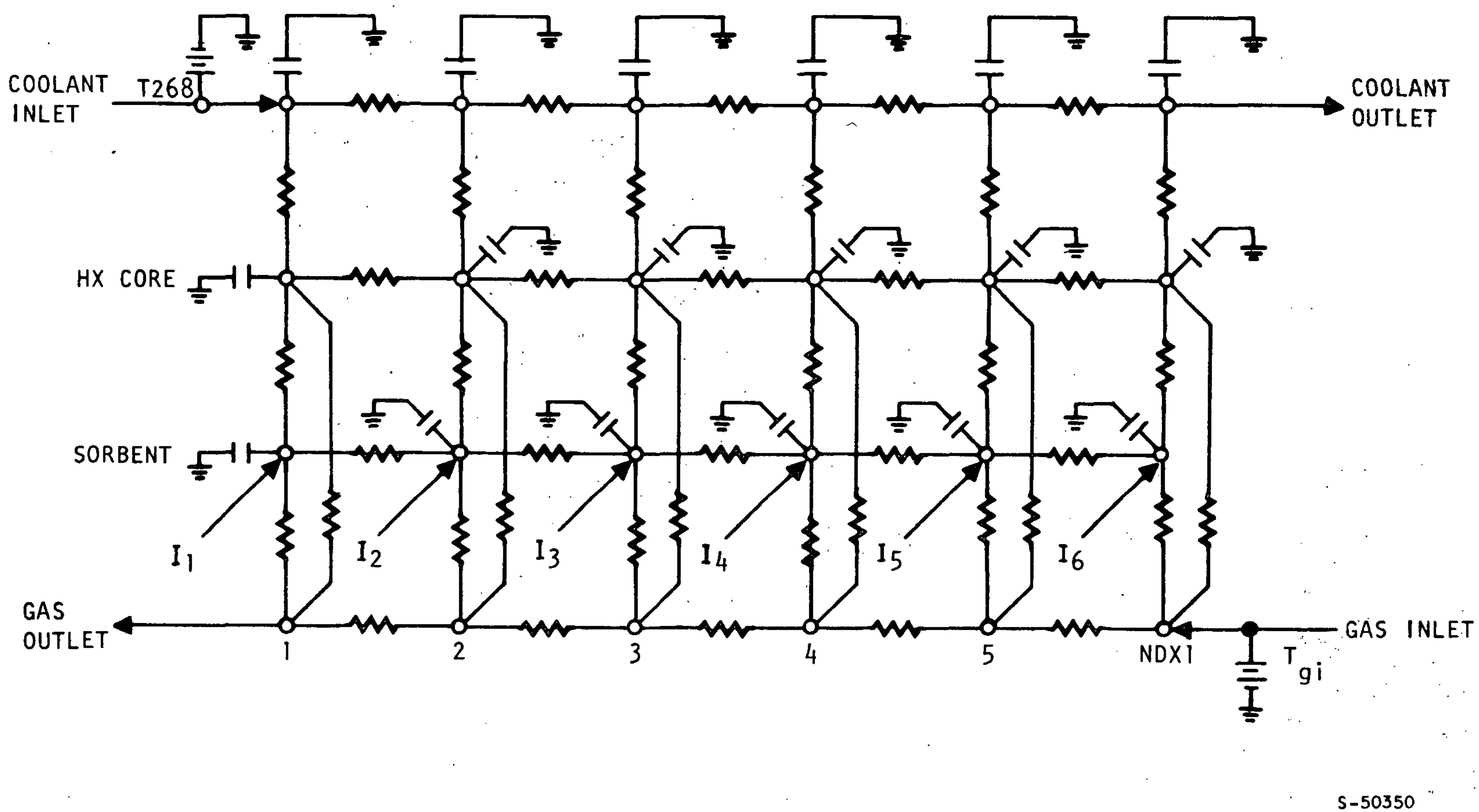

Figure 1-2. Thermal Network for Sorbent Bed During Adsorption

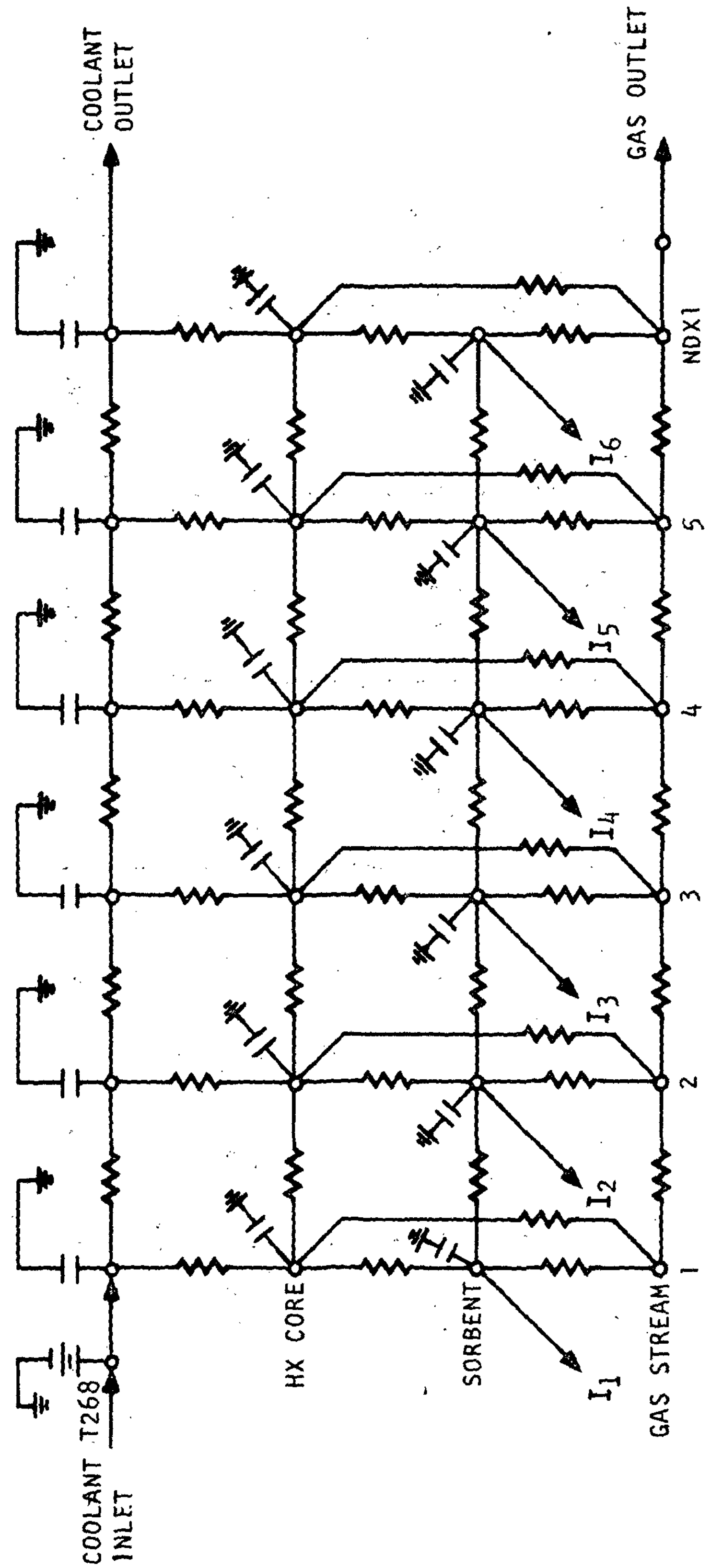

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Figure 1-3. Thermal Network for Sorbent Bed During Desorption

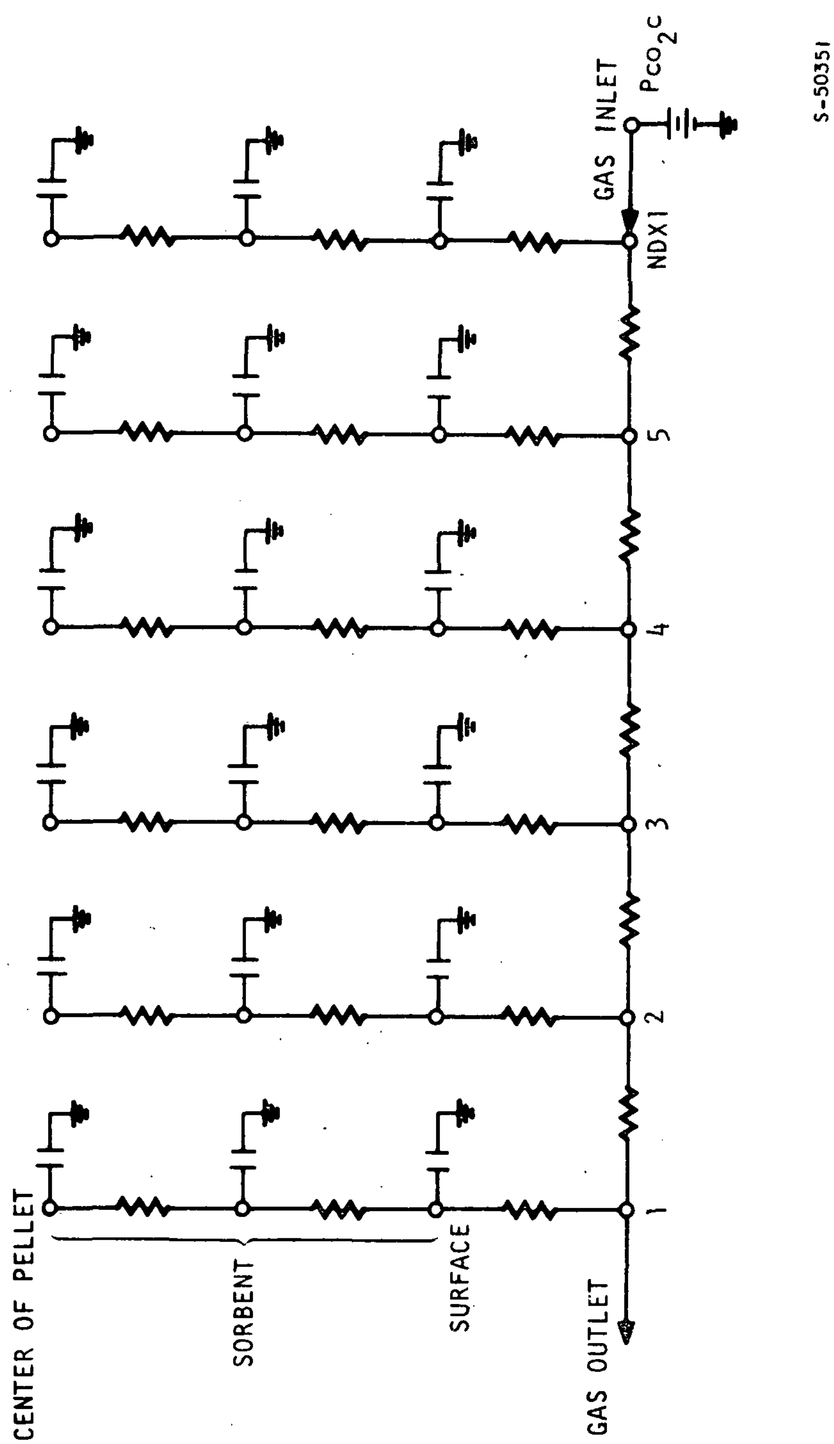

Figure 1-4. Mass Transfer Model for Sorbent Bed During Adsorption

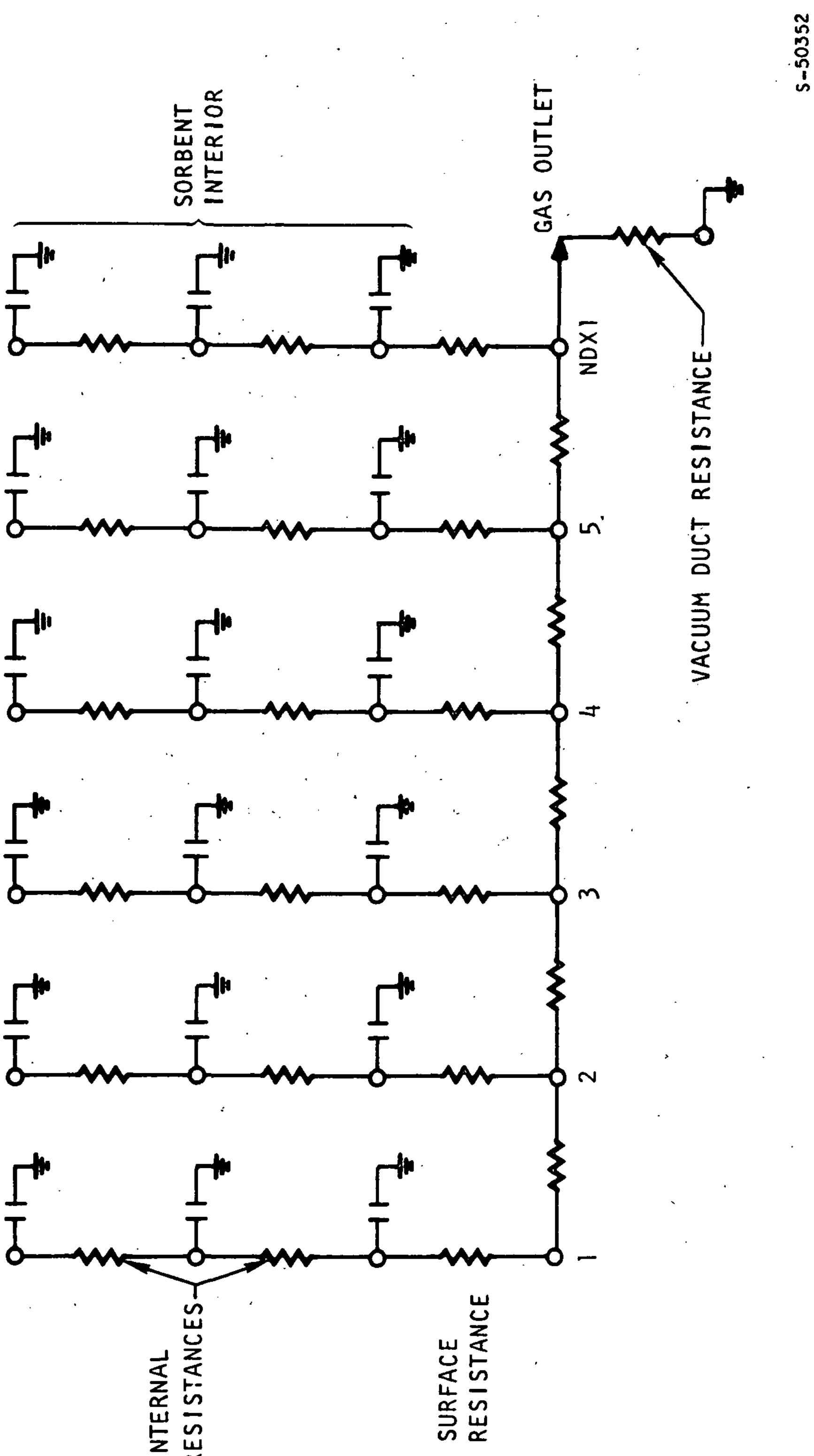

Figure 1-5. Mass Transfer Model for Sorbent Bed During Vacuum Desorption

specified performance requirements, if operating parameters are given. To optimize an entire vacuum-dump CO_2-removal system, the program can be used to generate curves showing the effects on total system weight of various parameters such as the process gas flow rate, bed size, coolant rate, and so forth. An optimum system can be easily found from that set of curves.

The program permits use of variable bed properties along the flow passage, and therefore, can be used for radial beds or beds of any arbitrary geometric configurations.

Input

The input to S9960 is by means of two BLOCK DATA subprograms, one for the adsorption period and the other for the desorption period computations. When running S9950 or S9951, only one pertinent BLOCK DATA subprogram is required.

In addition to the two block data subprograms, subprogram S9992 (PKEQ), which computes equilibrium vapor pressures of H_2O over the desiccant and CO_2 over the molecular sieve sorbent employed in the system, must be compiled with each run.

Output

Output from S9960 is the printed page. The output gives bed sizes, temperatures, sorbate loadings, partial pressures of CO_2 and H_2O during adsorption, total pressures during desorption, and average adsorption and desorption rates. Except at the end of each half cycle, the printout of bed properties will not appear until a number of adsorption-desorption cycles as specified by the input has been performed. The frequency of printout is also specified by the input.

Program Options

Various options available are summarized as follows:

- Use of S9950 for one half-cycle adsorption calculations
- Use of S9951 for one half-cycle desorption calculations
- Isothermal operation with the bed temperature specified
- Non-isothermal operation with the inlet coolant temperature specified
- Bed outlet pressure history during desorption inputted
- Bed outlet pressures computed from vacuum duct characteristics

- Bed cross-sectional areas vary in the axial direction
- Allowance of some inert nodes in the bed to simulate the case of partially poisoned bed
- Multi-outlet desorption with pressure history specified at up to three axial nodes

SECTION 2

TECHNICAL DESCRIPTION

GENERAL ASSUMPTIONS

In addition to some minor approximations that are presented under the derivation of equations, the following general assumptions were made in deriving the differential equations which were employed in the present program.

Assumption	Description
A	Temperature gradient in the pellet interior is negligible.
B	Adsorption occurs by the diffusion of an adsorbate through the stagnant surface film at the exterior surface of an adsorbent particle condensing at the surface and then diffusion into the interior of the particle. Desorption occurs in a reverse fashion.
C	Adsorbent pellets can be represented by spherical particles for mass transfer calculations.
D	Heats of adsorption and desorption do not depend on temperature or concentration.
E	In the adsorption half cycle, the total flow rate and density of the gas stream are constant.
F	Bed properties do not vary in the direction perpendicular to the direction of the gas flow.

DIFFERENTIAL MODEL

Only those equations that are not obvious will be given their derivations here. The equations which are assumed to be obvious or easily derived by the reader are listed with appropriate boundary conditions without proof. Initial conditions of the equations are omitted, since they should be apparent.

Diffusion Equation for Interior of Sorbent Pellet

$$\frac{\partial W_k}{\partial t} = \frac{D_k}{\rho_s} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial W_k}{\partial r} \right) \qquad (2\text{-}1)$$

Boundary conditions are

$$\frac{\partial W_k}{\partial r} = 0 \text{ at } r = 0 \tag{2-2}$$

$$-\rho_s D_k \frac{\partial W_k}{\partial r} = M_k K_g \left(P_{k_s} - P \cdot X_k\right) \text{ at } r = r_s \tag{2-3}$$

Energy Equation for Gas Stream

As the thermal capacitance of the gas in the void space of a sorbent bed is negligible compared with that of the sorbent bed or the heat exchanger core, a quasi-steady-state assumption can be made and the following is obtained, as energy equation for the gas stream,

$$\frac{dT_g}{dx} = \frac{1}{f \cdot \rho_g \cdot C_{pg} \cdot u_g} \left[a_{sg} \cdot h_{sg} \cdot (T_s - T_g) + a_{xg} \cdot h_{xg} \cdot (T_x - T_g)\right] \tag{2-4}$$

Equation (2-4) is subject to a boundary condition

$$T_g = T_{gi} \text{ at } x = x_o \text{ (i.e., process gas inlet)} \tag{2-5}$$

for the adsorption half cycle, while for the desorption half cycle, the condition to be satisfied is

$$T_g = T_s \text{ at } x = 0 \tag{2-6}$$

Energy Equation for Sorbent

$$\frac{\partial T_s}{\partial t} = \frac{\partial}{C_{ps}\rho_{sb}\partial x}\left(k_s A \frac{\partial T_s}{\partial x}\right) + \left(\frac{a_{sg} \cdot h_{sg}}{C_{ps} \cdot \rho_{sb}}\right)(T_g - T_s) + \left(\frac{a_{xs} \cdot h_{xs}}{C_{ps} \cdot \rho_{sb}}\right)(T_x - T_s)$$

$$+ \left(\frac{a_{sg} \cdot K_g}{C_{ps} \cdot \rho_{sb}}\right)(p_k - p_{ks}) \cdot (\Delta H_k) \tag{2-7}$$

This equation is subject to the conditions

$$\frac{\partial T_s}{\partial x} = 0 \text{ at } x = 0$$

$$\frac{\partial T_s}{\partial x} = 0 \text{ at } x = x_o \tag{2-8}$$

Energy Equation for Coolant Stream

$$\frac{\partial T_c}{\partial t} = -u_c \frac{\partial T_c}{\partial x} + \left(\frac{a_{vc} \cdot h_{xc}}{C_{pc} \cdot \rho_c}\right) (T_x - T_c) \qquad (2\text{-}9)$$

The boundary condition for this equation is

$$T_c = T_{268} \text{ at } x = x_{\text{coolant inlet}} \qquad (2\text{-}10)$$

Energy Equation for Heat Exchanger Core Metal

$$(C_{px} \cdot \rho_x) \frac{\partial T_x}{\partial t} = \frac{\partial}{\partial x}\left(k_x \frac{\partial T_x}{\partial_x}\right) + a_{vx} \cdot \Big[h_{xs} (T_s - T_x) + h_{xg} (T_g - T_x) + h_{xc} (T_c - T_x)\Big] \qquad (2\text{-}11)$$

Boundary conditions for this equation are

$$\frac{\partial T_x}{\partial x} = 0 \text{ at } x = 0 \text{ and } x = x_o \qquad (2\text{-}12)$$

Adsorption Material Balance Equation for k-th Component in Gas Stream

By neglecting axial diffusion and assuming that quasi-steady-state conditions exist for the gas phase material balance, the following is obtained.

$$\frac{dP_k}{dx} = \frac{P \cdot M_g}{f \cdot \rho_g \cdot u_g} \cdot a_{sg} \cdot K_g \cdot (p_{ks} - p_k) \qquad (2\text{-}13)$$

This has an inlet condition

$$p_k = p_{k,\text{inlet}} \text{ at } x = x_o \qquad (2\text{-}14)$$

Pressure Equation for Desorption

During the desorption cycle, both the bed pressure and gas flow rate vary with time and the axial location in the bed, and a method of calculating instantaneous pressures at various bed locations is desired. Although a quasi-steady-state assumption could be made regarding pressure calculations, the simplified problem obtained would still be a boundary value problem that requires an iterative method of solution. An alternative approach would be to solve a transient equation describing pressure changes. The latter approach was taken in the present program, and the derivation of the pressure-equation employed in the program is given below.

A material balance for a unit volume of bed gives

$$Af\left(\frac{\partial C}{\partial t}\right) = -\frac{\partial}{\partial x}(f \cdot C \cdot A \cdot u_g) + A \cdot \dot{M}_{sg} \quad (2\text{-}15)$$

where $$\dot{M}_{sg} = a_{sg} \cdot K_g \cdot (p_{ks} - P \cdot X_k) \quad (2\text{-}16)$$

and u_g is related to pressure gradient by

$$u_g = -\frac{1}{F}\left(\frac{\partial P}{\partial x}\right) \quad (2\text{-}17)$$

Also, by differentiating the perfect gas law

$$C = \frac{P}{RT_g} \quad (2\text{-}18)$$

one obtains

$$\frac{\partial C}{\partial t} = \frac{1}{RT_g}\left(\frac{\partial P}{\partial t}\right) - \left(\frac{P}{RT_g^2}\ \frac{\partial T_g}{\partial t}\right) \quad (2\text{-}19)$$

By combining Equations (2-17), (2-18), and (2-19), and dropping the term $\frac{P}{RT_g^2}\left(\frac{\partial T_g}{\partial t}\right)$, Equation (2-15) can be converted to Equation (2-20) in a quasi-isothermal condition:

$$\frac{\partial P}{\partial t} = \frac{P}{F}\left(\frac{\partial^2 P}{\partial x^2}\right) + \frac{P}{f \cdot C \cdot A}\ \frac{\partial}{\partial x}\left(\frac{A \cdot f \cdot C}{F}\right)\left(\frac{\partial P}{\partial x}\right) + \frac{P}{C \cdot f}\dot{M}_{sg} \quad (2\text{-}20)$$

Equation (2-20) is used in the program for calculating pressure changes during the desorption half cycle.

The proportionality constant F in Equation (2-17) is a strong function of pressure, as the gas flow during desorption lies in the slip flow region. The pressure drop data for the flow of nitrogen gas through a 5/8-in.-ID molecular sieve bed were reduced by using the equation

$$\frac{F_{N_2} G.R.T_g}{M_g} = \frac{\left(P_1^2 - P_2^2\right)}{2\,(x_2 - x_1)} \quad (2\text{-}21)$$

to obtain F_{N_2} at various mean pressures. The result is plotted in Figure 2-1 and a best straight line fit of the data gives

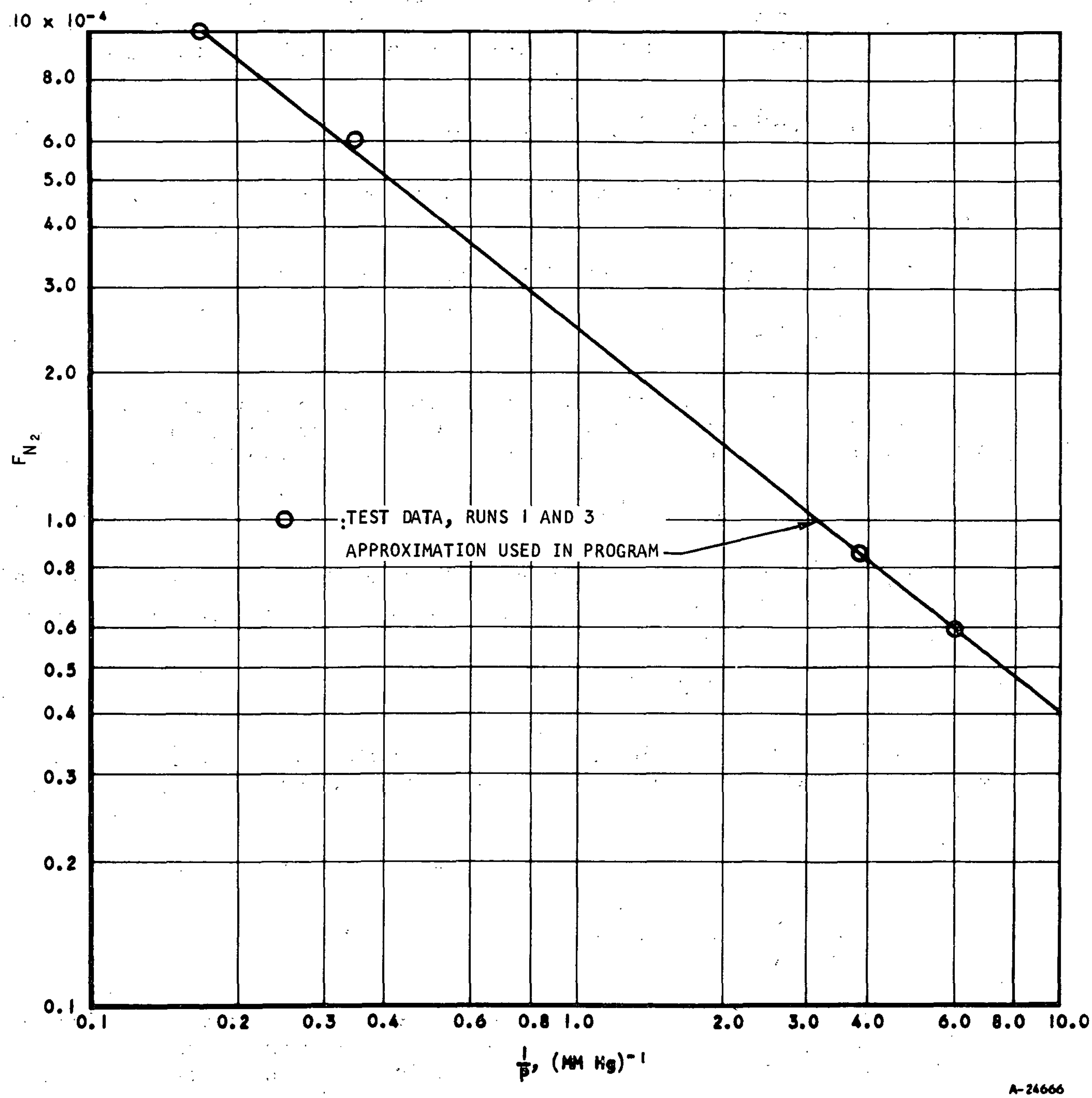

Figure 2-1. Correlation of F_{N_2} vs $(\frac{1}{P})$ From Test Data

$$F_{N_2} = 2.494 \times 10^{-4} \times P^{0.795} \tag{2-22}$$

Equation (2-22) is applicable only for nitrogen gas at 70°F, which has a viscosity of 0.0174 cp. In the desorption program, F is linearly corrected for the difference in viscosity as predicted by the Blake-Kozeny equation.

Thus $$F = \left(\frac{\text{Avg Viscosity}}{0.0174}\right) \cdot 2.494 \cdot 10^{-4} \cdot P^{0.795} \tag{2-23}$$

For the gas mixtures in the desiccant bed section, molal average viscosities were used in the program.

Equation (2-20) is subject to a boundary condition

$$\frac{\partial P}{\partial x} = 0 \text{ at } x = 0 \tag{2-24}$$

At the bed exit, the pressure can be specified as a function of time, or else the vacuum duct resistance to gas flow will play a role in fixing the pressure and flow rate. The boundary condition will then be

$$f \cdot \rho_g \cdot u_g \cdot A = W_D(P) \tag{2-25}$$

where $W_D(P)$ can be approximated by the following expression which corresponds to the straight line shown in Figure 2-2 for a 3-in. duct for the AAP vacuum duct.

$$W_D(P) = 11.2\ P^{1.715} \tag{2-26}$$

The dotted lines in Figure 2-2 were the estimated flow rates for 18 in. long ducts. The resistance contributed by the gas valve were not included in these calculations.

Combination of Equations (2-17), (2-25), and (2-26) yields

$$\frac{\partial P}{F \partial x} = \left(\frac{11.2\ P^{0.715}}{f \cdot \rho_g \cdot A}\right) P \tag{2-27}$$

In addition to the equations listed above, an equilibrium relationship between vapor pressure, temperature, and sorbate loading is needed for each sorbate-sorbent combination. The relationship can be in equation or tabular form.

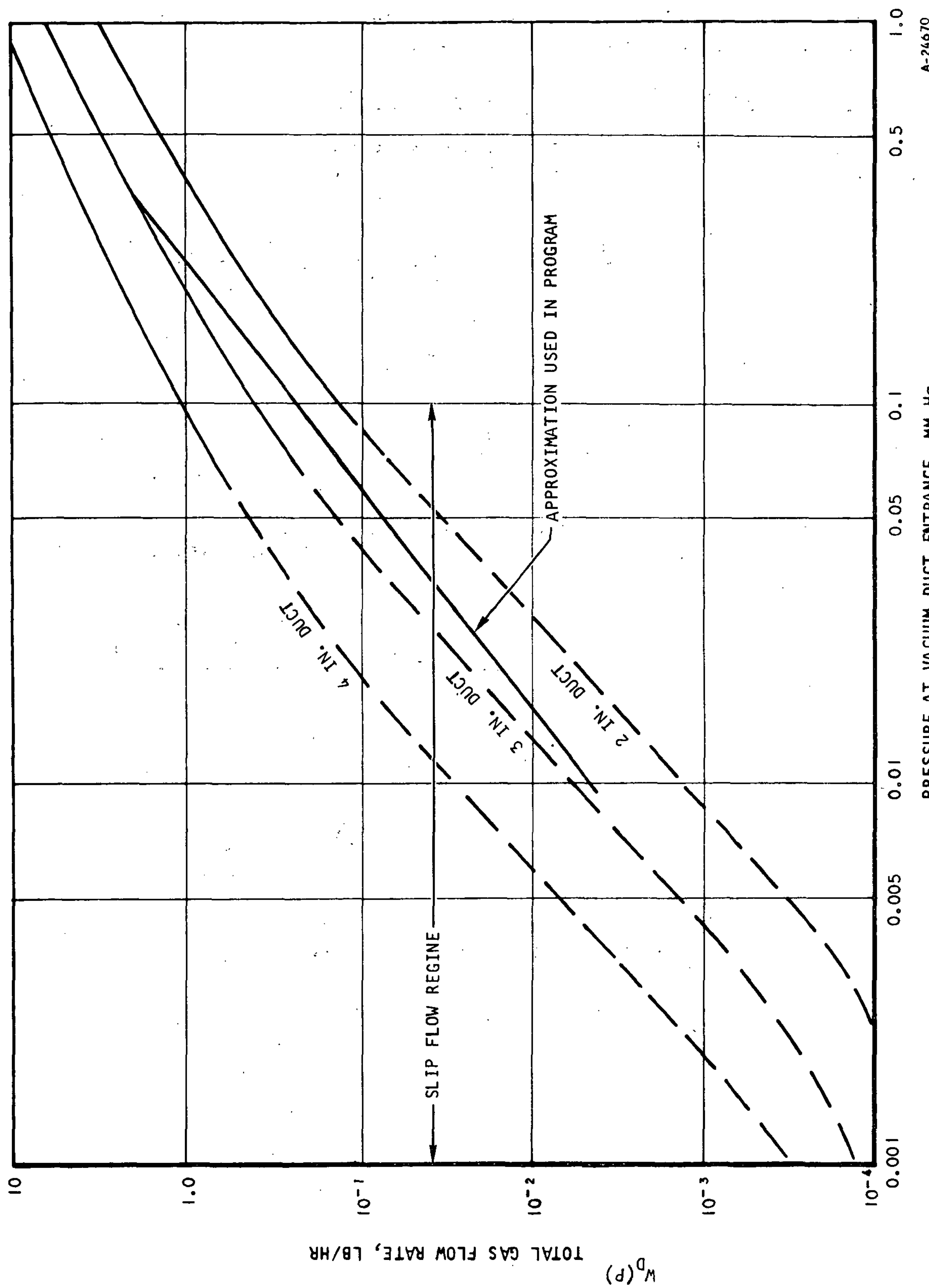

Figure 2-2. Vacuum Duct Capacities for Various Duct Sizes and Duct Inlet Pressures

FINITE DIFFERENCE MODEL

The foregoing differential equations were solved in the program, using the following finite-difference approximations.

Diffusion Equation for Interior of Sorbent Pellet

For accuracy, the sorbent is divided into constant volume elements rather than into ones with constant (Δr). Equation (2-1) can then be approximated by

$$(\Delta V)\rho_s \cdot \left[\frac{W_{k,M,(t+\Delta t)} - W_{M,k,t}}{(\Delta t)}\right] = \rho_s D_k \cdot \frac{\left(4\pi \cdot r^2_{M-1/2}\right)}{(r_M - r_{M-1})} \tag{2-28}$$

$$\cdot \left(W_{k_{(M-1)(t+\Delta t)}} - W_{k_{M,(t+\Delta t)}}\right)$$

$$- \frac{\rho_s \cdot D_K \left(4\pi r^2_{M+1/2}\right)}{(r_{M+1} - r_M)} \cdot \left(W_{k_{M,(t+\Delta t)}} - W_{k_{(M+1)(t+\Delta t)}}\right)$$

Half nodes are used at the center and the surface of spherical pellets, and Equation (2-28), with boundary conditions (2-2) and (2-3) super imposed becomes respectively

$$\frac{(\Delta V)}{2} \cdot \rho_s \frac{W_{k,1(t+\Delta t)} - W_{k,1(t+\Delta t)}}{(\Delta t)} = - \frac{\rho_s D_k \left(4\pi r^2_{1-1/2}\right)}{(r_2 - 0)} \tag{2-29}$$

$$\left[W_{k,1,(t+\Delta t)} - W_{k,2,(t+\Delta t)}\right]$$

and

$$\frac{(\Delta V)}{2} \cdot \rho_s \frac{W_{k,s,(t+\Delta)} - W_{k,s,t}}{(\Delta t)} = - \frac{\rho_s D_K \left(4\pi \cdot r^2_{M_s - 1/2}\right)}{r_s - r_{M_s - 1}} \cdot \tag{2-30}$$

$$\left[W_{k,(M_s-1),(t+\Delta t)} - W_{k,M_s,(t+\Delta t)}\right]$$

$$-A_s \cdot M_k \cdot K_g \cdot \left(p_{ks} - P \cdot X_k\right)_{(t+\Delta t)}$$

Energy Equation for Gas Stream

Equation (2-4) is approximated by

$$\frac{T_{g(N+1)} - T_{g(N)}}{(\Delta x)} = \frac{1}{f \cdot \rho_g \cdot C_{pg} \cdot u_g} \left[a_{sg} \cdot h_{sg} \cdot \left(T_{s(N+1)} - T_{g(N+1)} \right) + a_{xg} \cdot h_{xg} \left(T_{x(N+1)} - T_{g(N+1)} \right) \right] \tag{2-31}$$

for $u_g > 0$

For the case $u_g < 0$, which is the case during adsorption, the index (N+1) will be replaced by (N-1).

Energy Equation for Sorbent

The following finite difference representation for Equation (2-7) is used in the program.

$$\frac{T_{s(t+\Delta t),N} - T_{s(t-\Delta t),N}}{2 \cdot (\Delta t)} = \frac{1}{C_{ps} \cdot \rho_{sb} \cdot (\Delta x)^2 A_N} \cdot \Big[k_{s(N+1/2)} \cdot A_{(N+1/2)} \cdot \left(T_{s(t+\Delta t),(N+1)} - T_{s(t+\Delta t),N} \right) - k_{s(N-1/2)} \cdot A_{(N-1/2)} \cdot \left(T_{s(t+\Delta t),N} - T_{s(t+\Delta t),(N-1)} \right) \Big] + \left(\frac{a_{sg} \cdot h_{sg}}{C_{ps} \cdot \rho_{sb}} \right)_N \cdot \left[T_{g_{t,N}} - \frac{T_{s(t+\Delta t),N} + T_{s(t-\Delta t),N}}{2} \right] + \left(\frac{a_{xs} - h_{xs}}{C_{ps} \cdot \rho_{sb}} \right)_N \left[T_{x_{t,N}} - \frac{T_{s(t+\Delta t),N} + T_{s(t-\Delta t),N}}{2} \right] + \left(\frac{a_{sg} \cdot K_g}{C_{ps} \cdot \rho_{sb}} \right)_N \cdot \left[P_{k(t+\Delta t),N} - P_{ks(t+\Delta t),N} \right] \cdot (\Delta H_k) \tag{2-32}$$

Energy Equation for Coolant Stream

The program uses the finite-difference analog to Equation (2-9)

$$\frac{T_{c_{(t+\Delta t),N}} - T_{c_{(t-\Delta t),N}}}{2(\Delta t)} = -u_c \frac{T_{c_{(t+\Delta t),N}} - T_{c_{(t+\Delta t),(N-1)}}}{(\Delta x)} \tag{2-33}$$

$$+ \left(\frac{a_{vc} \cdot h_{xc}}{C_{pc} \cdot \rho_c}\right)_N \cdot \left[T_{x_{t,N}} - \frac{T_{c_{(t+\Delta t),N}} + T_{c_{(t-\Delta t),N}}}{2}\right]$$

Energy Equation for Heat-Exchanger Core Metal

$$(C_{px} \cdot \rho_x) \frac{T_{x_{(t+\Delta t),N}} - T_{x_{(t-\Delta t),N}}}{2 \cdot (\Delta t)} = \frac{1}{(\Delta x)^2} \cdot \left[k_{x_{(N+1/2)}}\right. \tag{2-34}$$

$$\cdot \left(T_{x_{(t+\Delta t),(N+1)}} - T_{x_{(t+\Delta t),N}}\right) - k_{x_{(N-1/2)}} \left(T_{x_{(t+\Delta t),N}}\right.$$

$$\left.\left. -T_{x_{(t+\Delta t),(N-1)}}\right)\right] + a_{vx} \cdot h_{xs}$$

$$\cdot \left\{T_{s_{t,x}} - \frac{T_{x_{(t+\Delta t),N}} + T_{x_{(t-\Delta t),N}}}{2}\right\} + h_{xg} \cdot \left\{T_{g_{t,N}}\right.$$

$$\left. - \frac{T_{x_{(t+\Delta t),N}} + T_{x_{(t-\Delta t),N}}}{2}\right\} + h_{xc} \cdot \left\{T_{c_{t,N}}\right.$$

$$\left.\left. - \frac{T_{x_{(t+\Delta t),N}} + T_{x_{(t-\Delta t),N}}}{2}\right\}\right]$$

Adsorption Material Balance for K-th Component in Gas Stream

Equation (2-13) is approximated by

$$\frac{p_{k_{(N-1)}} - p_{k_{(N)}}}{(\Delta x)} = \left(\frac{P \cdot M_g}{f \cdot \rho_g \cdot u_g}\right) \cdot a_{sg} \cdot k_g \cdot \left(p_{ks_{(N-1)}} - p_{k_{(N-1)}}\right) \tag{2-35}$$

Pressure Equations for Desorption

Equation (2-20) is represented by

$$\frac{P_{(t+\Delta t),N} - P_{t,N}}{(\Delta t)} = \frac{P_{t,N}}{F_{t,N} \cdot (\Delta x)^2} \Big[P_{(t+\Delta t),(N-1)} - 2P_{(t+\Delta t),N} \tag{2-36}$$

$$+ P_{(t+\Delta t),(N+1)}\Big] + \left(\frac{P}{f \cdot C \cdot A}\right)_{t,N} \cdot \frac{1}{2(\Delta x)^2}$$

$$\left[\left(\frac{A \cdot f \cdot C}{F}\right)_{t,N} - \left(\frac{A \cdot f \cdot C}{F}\right)_{t,(N-1)}\right] \cdot \left[P_{(t+\Delta t),(N+1)} - P_{(t+\Delta t),(N-1)}\right]$$

$$+ \left(\frac{P}{C \cdot f}\right)_{t,N} \cdot a_{sg} \cdot K_g \cdot \left[P_{ks_{(t+\Delta t),N}} - P_{(t+\Delta t),N} \cdot X_{k_{t,N}}\right]$$

The boundary condition expressed by Equation (2-27) can be put in the form

$$-\frac{P_{(NDXI+1)} - P_{NDXI}}{F \cdot (\Delta x)} = \left(\frac{11.2\ P^{0.715}}{f \cdot \rho_g \cdot A}\right)_{NDXI} P_{NDXI} \tag{2-37}$$

METHOD OF SOLUTION

Most of the finite difference schemes described above are of the implicit form and require a special method of solution, which is described below.

The system of finite difference equations describing bed property changes for all nodes can be written in the form (Reference 3)

$$C_{2_1} Y_{1,(t+\Delta t)} + C_{3_1} Y_{2,(t+\Delta t)} = D_1 \tag{2-38}$$

$$C_{1_N} Y_{(N-1),(t+\Delta t)} + C_{2_N} Y_{N,(t+\Delta t)} + C_{3_N} Y_{(N+1),(t+\Delta t)} = D_N \tag{2-39}$$

$$C_{1_{NDXI}} Y_{(NDXI-1),(t+\Delta t)} + C_{2_{NDXI}} Y_{(NDXI),(t+\Delta t)} = D_{NDXI} \tag{2-40}$$

The matrix of this linear system is tridiagonal and the following formulae which were first presented by Thomas,[2] are used for its solution:

$$B_1 = \frac{C_{3_1}}{C_{2_1}} \tag{2-41}$$

$$B_N = \frac{C_{3_N}}{\left(C_{2_N} - C_{1_N} B_{N-1}\right)} \quad (N = 2, 3, \ldots, NDX1) \tag{2-42}$$

$$Q_1 = \frac{D_1}{C_{2_1}} \tag{2-43}$$

$$Q_N = \frac{\left(D_N - C_{1_N} Q_{N-1}\right)}{\left(B_N - C_{1_N} B_{N-1}\right)}, \quad (N = 2, 3, \ldots, NDX1) \tag{2-44}$$

$$Y_{NDX1} = Q_{NDX1} \tag{2-45}$$

$$Y_N = Q_N - B_N Y_{N+1}, \quad [N = (NDX1-1), (NDX1-2), \ldots, 1) \tag{2-46}$$

It should be noted that the index N appearing in the above equations can be replaced by index M for solving the interior diffusion Equation (2-28) with its boundary conditions.

Equation (2-35) for the adsorption period and Equation (2-36) for the desorption period are coupled with Equations (2-30) and (2-32) and a special method is needed, which is described below for the desorption period first because this is the more involved of the two cases.

Equilibrium surface vapor pressure at the end of a time step is approximated by

$$P_{k,s,(t+\Delta t)} = P_{k,s,t} + \left(W_{k,s,(t+\Delta t)} - W_{k,s,t}\right) \left(\frac{\partial p_k^*}{\partial W_k}\right)_{T_s} + \left(T_{s,(t+\Delta t)} - T_{s,t}\right) \left(\frac{\partial p_k^*}{\partial T_s}\right)_{W_{k,s}} \tag{2-47}$$

The new surface loading can be expressed as a function of the gas phase pressure:

$$W_{k,s,(t+\Delta t)} = Q_s + D_2 \cdot P_{(t+\Delta t)} \tag{2-48}$$

where Q_s is the Q as expressed by Equation (2-44) for the pellet interior diffusion, with the term containing $P_{(t+\Delta t)}$ excluded from it.

Sorbent temperature change in one time step during the desorption period is written as:

$$T_{s,(t+\Delta t)} - T_{s,t} = D_s + C_{s1} \cdot P_{(t+\Delta t)} - C_{s2} \cdot p_{k,s(t+\Delta t)} \tag{2-49}$$

Substituting Equations (2-48) and (2-49) into Equation (2-47), the following is obtained

$$p_{k,s,(t+\Delta t)} = P_1 + P_2 \left[Q_s - W_{k,s,t}\right] + \left[P_2 \cdot D_2 + P_3\right] \cdot P_{(t+\Delta t)} \tag{2-50}$$

where

$$P_1 = \left[p_{k,s,t} + D_s \left(\frac{\partial p_k^*}{\partial T_s}\right)_{W_k}\right] \Bigg/ \left[1 + C_{s2} \cdot \left(\frac{\partial p_k^*}{\partial T_s}\right)_{W_k}\right] \tag{2-51}$$

$$P_2 = \left(\frac{\partial p_k^*}{\partial W_k}\right)_{T_s} \Bigg/ \left[1 + C_{s2}\left(\frac{\partial p_k^*}{\partial T_s}\right)_{W_k}\right] \tag{2-52}$$

$$P_3 = C_{31} \cdot \left(\frac{\partial p_k^*}{\partial T_s}\right)_{W_k} \Bigg/ \left[1 + C_{s2} \left(\frac{\partial p_k^*}{\partial T_s}\right)_{W_k}\right] \tag{2-53}$$

Now, Equation (2-36) can be rewritten as follows, where N designates the N-th axial node counted from the furthest end from the vacuum duct connection:

$$\frac{P_{N,(t+\Delta t)} - P_{N,(t)}}{(\Delta t)} = P_{C1} \cdot \frac{P_{(N-1),(t+\Delta t)} - 2 \cdot P_{N,(t+\Delta t)} + P_{(N+1),(t+\Delta t)}}{(\Delta x)^2}$$

$$+ P_{C2} \cdot \frac{P_{(N+1),(t+\Delta t)} - P_{(N-1),(t+\Delta t)}}{2 \cdot (\Delta x)} \tag{2-54}$$

$$+ P_{C3} \cdot \left[p_{ks} - X_k \cdot P_{N,(t+\Delta t)}\right]$$

The last term of this equation becomes, by the substitution of Equation (2-50):

$$P_{C3} \cdot \left[p_{ks} - X_k \cdot P_{N,(t+\Delta t)}\right] = C_{P1_N} + C_{P2_N} \cdot P_{N,(t+\Delta t)} \tag{2-55}$$

where $$C_{P1_N} = P_{C3_N} \cdot \left[P_{1_N} + P_{2_N} \cdot \left\{ Q_{s_N} - W_{k_{s(t)}} \right\} \right] \quad (2\text{-}56)$$

$$C_{P2_N} = P_{C3_N} \cdot \left[\left\{ P_{2_N} \cdot D_{2_N} + P_{3,N} \right\} - X_k \right] \quad (2\text{-}57)$$

Combining Equations (2-54) and (2-55) and rearranging, the following is obtained.

$$C_{1P,N} \cdot P_{(N-1),(t+\Delta t)} + C_{2P,N} \cdot P_{N,(t+\Delta t)} + C_{3P,N} \quad (2\text{-}58)$$

$$\cdot P_{(N+1),(t+\Delta t)} = D_{1P,N}$$

where $$C_{1P,N} = -\frac{P_{C1,N}}{(\Delta x)^2} + \frac{P_{C2,N}}{2 \cdot (\Delta x)} \quad (2\text{-}59)$$

$$C_{2P,N} = \frac{1}{(\Delta t)} + \frac{2 \cdot P_{C1,N}}{(\Delta x)^2} - C_{P2,N} \quad (2\text{-}60)$$

$$C_{3P,N} = \frac{P_{C1,N}}{(\Delta x)^2} - \frac{P_{C2,N}}{2(\Delta x)} \quad (2\text{-}61)$$

$$D_{1P,N} = \frac{P_{N,t}}{(\Delta t)} + C_{P1,N} \quad (2\text{-}62)$$

Equation (2-58) has P as the only unknown, and can be solved by the method using Equations (2-41) through (2-46). Once P's are found, new loadings and temperatures can be obtained using these pressures.

For the adsorption period, by setting $X_k = 1$, and replacing P by p_k, Equation (2-36) by Equation (2-35), the following equations are obtained:

$$W_{ks,(t+\Delta t)} = Q_s + D_2 \cdot p_{k(t+\Delta t)} \quad (2\text{-}64)$$

$$T_{s,(t+\Delta t)} - T_{s,t} = D_s + C_{s1} \cdot p_{k,(t+\Delta t)} - C_{s2} \cdot p_{k,s,(t+\Delta t)} \quad (2\text{-}65)$$

$$p_{k,s,(t+\Delta t)} = P_1 + P_2 \left[Q_s - W_{k,s,t} \right] + \left[P_2 \cdot D_2 + P_3 \right] \quad (2\text{-}66)$$

$$\cdot p_{k,(t+\Delta t)}$$

$$p_{k,N,(t+\Delta t)} = \left[\frac{p_{k,(N+1),(t+\Delta t)}}{(\Delta x)} + \frac{C_{P1,N}}{\frac{f \rho_g \cdot u_g}{P \cdot M_g}} \right] \Bigg/ \left[\frac{1}{(\Delta x)} - \frac{C_{P2,N}}{\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g}\right)} \right] \tag{2-67}$$

where

$$C_{P1,N} = a_{sg} \cdot K_g \cdot \left[P_1 + P_2 \cdot (Q_s - W_{k,s}) \right] \tag{2-68}$$

$$C_{P2,N} = a_{sg} \cdot K_g \cdot (P_2 \cdot D_2 + P_3 - 1) \tag{2-69}$$

Equation (2-67) is used to find p_k's from the process gas inlet end all the way to the outlet end. W_k's are found next, followed by temperatures.

GENERAL FLOW CHART

A general flow diagram of S9960 is given in Figure 2-3.

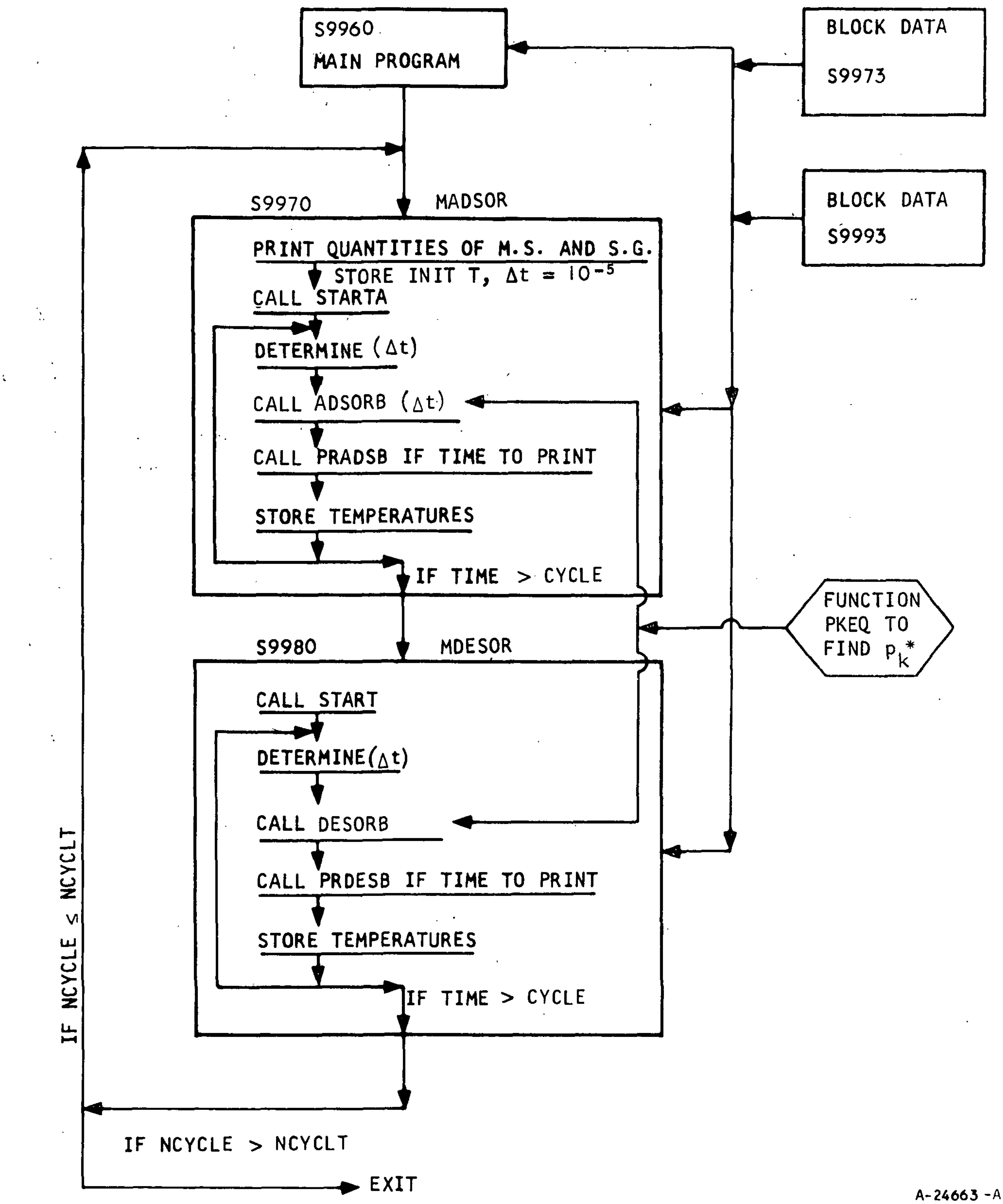

Figure 2-3. Structure of Program S9960

SECTION 3

USAGE

PROGRAM INPUT

Data input required by the program is executed by block data subprograms S9973 and S9993. Subprogram S9973 inputs all data required to execute the adsorption analysis; subprogram S9993 inputs all data required to execute the desorption analysis. Both block data subprograms must be compiled at execution time if cyclic system performance is desired. If only adsorption or desorption performance is required, then only the respective block data subprogram need be compiled at execution time. The following lists the variables which are inputted via the block data subprograms.

Variables Common to Both S9973 and S9993

FORTRAN Symbol	Maximum Dimension	Definition
		Bed Configuration
ABED	(41)	Sorbent bed cross-section area normal to flow of process gas, sq ft
AGX	(41)	Identical to ASX
ASX	(41)	Heat exchanger primary area per unit volume of sorbent bed, sq ft/(cu ft)
DX		Axial node dimension, ft
NDR4		Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDXM		Integer denoting total number of modecular sieve nodes
NDXMAC		Integer denoting number of active molecular sieve nodes, i.e., (NDXM - NDXMAC) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NDX1		Integer denoting total number of axial nodes

FORTRAN Symbol	Maximum Dimension	Definition
		Sorbent Properties
ASG	(41)	Sorbent specific surface area, sq ft/(cu ft of bed)
CPS	(41)	Sorbent specific heat, Btu/(lb) (°F)
RHOS	(2)	Sorbent particle density, lb/(cu ft) RHOS (1) = molecular sieve particle density, RHOS (2) = desiccant particle density
RHOSB	(41)	Sorbent bulk density, lb/(cu ft)
SK	(41)	Effective sorbent thermal conductivity, Btu/(hr) (sq ft) (°F/ft)
		Coolant Properties
AVC	(41)	Primary heat exchanger plate area per unit volume of coolant held up in HX, sq ft/(cu ft)
CPC	(41)	Coolant specific heat, Btu/(lb) (°F)
NOG		Node to which coolant is added
RHOC	(41)	Coolant density, lb/(cu ft)
T268		Coolant inlet temperature, °F
UC	(41)	Coolant velocity, ft/hr
		Heat Transfer Coefficients
HSG	(41)	Heat transfer coefficient, sorbent to gas, Btu/(hr) (sq ft)(°F)
HXC	(41)	Heat transfer coefficient,heat exchanger to coolant Btu/(sq ft) (hr)(°F)
HXG	(41)	Heat transfer coefficient, heat exchanger to process gas, Btu/(sq ft) (°F) (hr)
HXS	(41)	Heat transfer coefficient, heat exchanger to sorbent, Btu/(sq ft)(hr)(°F)

FORTRAN Symbol	Maximum Dimension	Definition
		Initial Conditions
TC	(41)	Initial coolant temperature, °F
TG	(41)	Initial gas temperature, °F
TS	(41)	Initial sorbent temperature, °F
TX	(41)	Initial heat exchanger temperature, °F
W	(21,41)	Initial sorbent loading, lb/lb (double precision)
		Mass Transfer Properties
DIF	(41)	Internal diffusivity, sq ft/hr
GK	(41)	External surface mass transfer coefficient, lb-mole/(hr)(sq ft)(mm Hg)
		Process Gas Stream Properties
CPG	(41)	Specific heat of the process gas, Btu/(lb)(°F)
DH	(41)	Differential heat of adsorption, Btu/(lb adsorbed)
WM	(2)	Adsorbate molecular weight WM(1) = 44 (CO_2) WM(2) = 18 (H_2O)
		HX Core Properties
AVX	(41)	Primary heat exchanger plate area per unit volume of heat exchanger core metal, sq ft/(cu ft)
CPX	(41)	Heat exchanger specific heat, Btu/(°F)(lb)
RHOX	(41)	Heat exchanger metal density, lb/(cu ft)
TKX	(41)	Heat exchanger metal thermal conductivity, TKX (K) denotes that between node K-1 and node K, Btu/(hr)(sq ft)(°F/ft)

FORTRAN Symbol	Maximum Dimension	Definition
		Miscellaneous Control Parameters
CYCLE		Cycle time per one adsorption or one desorption, period, hr
DTMAX		Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
NCYCLT		Total number of complete adsorption-desorption cycle calculations desired
NDTCØN		If NDTCØN = 1, Δt will be selected such that ΔT = TI, ΔW = WI for time step; if NDTCØN = 2, Δt's as set in program will be used
NPRINT		Integer control variable which determines the frequency of printout occurrence; e.g., if NPRINT = 2, printout occurs after every two time steps, if NPRINT = 5, printout occurs after every five time steps,etc.
NTEMP		Integer control variable; if NTEMP = 0, isothermal analysis; the energy equations are ignored, and the bed temperature is set equal to T268. If NTEMP ≠ 0, nonisothermal analysis
TI		Maximum temperature change allowable per time increment in selecting Δt, ^{o}F
WI		Maximum loading change allowable per time increment in selecting Δt, lb/lb

NOTE: Variables W, TG, TS, TC, TX, NPRINT, DTMAX, NTEMP, CYCLE, NCYCLT, WI, TI, NDXMAC and NDTCØN need to appear only once either in S9973 or S9993.

Input Variables Required by S9973 Only

FORTRAN Symbol	Definition
GMR	Process gas flow rate, lb/hr
GMW	Process gas molecular weight
PA	System total pressure, mm Hg
PCØ2C	Initial CO_2 partial pressure in cabin, mm Hg
PH2Ø1	Inlet H_2O partial pressure, mm Hg
TGI	Inlet process gas temperature, ^{0}F
VØLCAB	Cabin volume for atmosphere, cu ft; use VØLCAB = 10^{20}, for constant PCØ2C
RCØ2C	Rate of CO_2 generation in cabin, lb CO_2 per hr

Input Variables Required by S9993 Only

FORTRAN Symbol		Definition
NBCOUT		Integer control variable; if NBCOUT = 2, the outlet manifold pressure is specified as a function of time; NBCOUT = 1, the manifold pressure is computed from vacuum duct resistance
POUT TIMET	(10) (10)	10 pairs of exit pressure vs time data to be used if NBCOUT = 2; POUT = vacuum end manifold pressures (mm Hg), TIMET = times (hr)
NPSET	(3)	Denotes nodes to which vacuum is applied

Function PKEQ (ID, W,T), S9992

This function subprogram must be defined, which computes for ID = 1, the equilibrium CO_2 pressure over the molecular sieve sorbent at a loading of W lb CO_2/lb sieve and at T ^{0}F; and for ID = 2, computes H_2O vapor pressure over the desiccant sorbent at a loading of W lb H_2O/lb desiccant and T ^{0}F.

Equilibrium isotherms can be used in tabular forms and $p_k^*{}_{(W,T)}$ obtained by an interpolation technique, or the data can be fit by a mathematical expression which is evaluated in this subprogram. The latter approach is recommended since experience has indicated that by using the former approach, the total run time of the present program is about twice the time required by using the latter approach.

Vacuum Duct Characteristics

The vacuum duct characteristics represented by Equation (2-26) was for a 3-in.-ID by 18 in. long duct, which may not be the case for the problem to be simulated. If this is the case the outlet boundary condition expressed by Equations (2-26) and (2-37) must be modified. The required changes are minor and will be shown in the example problem to be presented in Section 4.

OUTPUT DESCRIPTION

The first page of output gives bed volumes and weights of molecular sieves and desiccants.

From the second page on, bed properties are printed at the end of each adsorption and desorption period. From the NSTART-th cycle on, the bed properties are printed every NPRINT time steps.

In the adsorption period, the cycle number is printed on the first line. Time from the beginning of adsorption period is printed next in hours and minutes. The size of time increment last used follows the adsorption time. CO_2 and H_2O partial pressures in the process gas stream, gas, sorbent, coolant, and HX core temperatures are then given at each axial node, node 1 designating the bed outlet and the highest node representing the process gas inlet node. Sorbate loadings in (lb sorbate)/(lb sorbent) appear at all sorbent interior nodes and at all axial locations. The average loading at each axial location is also given. The average CO_2 loading in the active molecular sieve sorbent, the average H_2O loading in the desiccant sorbent, average rates of CO_2 and H_2O adsorption computed over the period from the beginning of the adsorption cycle up to the moment, time average water partial pressure at the bed outlet, and the average rate of H_2O influx into the CO_2-sorbent section are printed.

Printouts during desorption periods are similar to those of adsorption periods except that, for all longitudinal locations total pressures instead of the partial pressures of CO_2 and H_2O are printed, and in addition, mole fractions of H_2O in the vapor phase and molal flow rates of CO_2 and H_2O for all axial nodes, are also written.

EXECUTION CHARACTERISTICS

Restrictions

The program is limited in the case where sorbents are regenerated by vacuum desorption, either with or without the application of heat in addition. Program modifications will be required if gas stripping is resorted for sorbent regenerations.

The program requires a total of 31,000 words storage with Univac 1108 computer.

Running Time

Running time depends on the total number of nodes employed in a simulation. Using a total of 18 nodes, the ratio of real time to Univac 1108 computer time is roughly 150 to 1.

Accuracy/Validity

The present program was tested on the regenerable CO_2 removal systems for AAP and Airlock applications. Comparisons between the predictions made by the program and the test data are reasonably good.

SECTION 4

SAMPLE PROBLEM SOLUTION

BED DESIGN

As an example of the program usage, the performance of the CO_2-removal system designed by AiResearch for the Airlock application will be simulated. The bed design is shown in Figure 4-1.

The predryer section is bulk packed with Linde Molecular Sieves type 13X of 1/16 in. size. The CO_2 adsorber is composed of an electrically heated plate-fin heat exchanger, with the gas passages filled up with Linde Molecular Sieves type 5A of 1/16 in. size. The electric heater is used only for bakeout, and during normal operation the heat exchanger, together with the heater, simply acts as a thermal capacitor only. The electric heater elements used are KAPTON and the plate-fin heat exchanger is aluminum. The outside shell of the canister is made of stainless steel.

DESCRIPTION ON GENERATION OF INPUT DATA

The input data for simulating the performance of the above CO_2 removal unit are described below. Since no coolant is used for temperature control in the present system, coolant nodes are used as ambient temperature nodes to simulate heat losses to the surroundings, and the thermal capacitance of the heater is lumped into sorbent nodes. Heat exchanger core metal nodes designate the shell temperatures.

Bed Configuration

AVX = 375.0 is obtained by dividing the shell area by shell volume

ASX = AGX = 6.18 is obtained by dividing shell area by bed volume

ASG = 700 for bulk packed 1/16 in. pellets,

= 560 for same pellets in heat exchanger section

Heat Transfer Coefficients

1. Sorbent to Gas

HSG = 20 during adsorption. This is obtained from the low Reynolds number calculations of Pfeffer (Reference 4). The Nusselt number with a flow rate of 10.0 lb/hr is about 8.2. With a gas phase thermal conductivity of 0.01475 $\frac{\text{Btu}}{\text{hr ft}^{\circ}\text{F}}$ and an effective particle diameter of:

$$d = \frac{6 \times 45}{64 \times 700} = 0.00603 \text{ ft},$$

MOLECULAR SIEVE CANISTER COMPUTER NODAL STRUCTURE

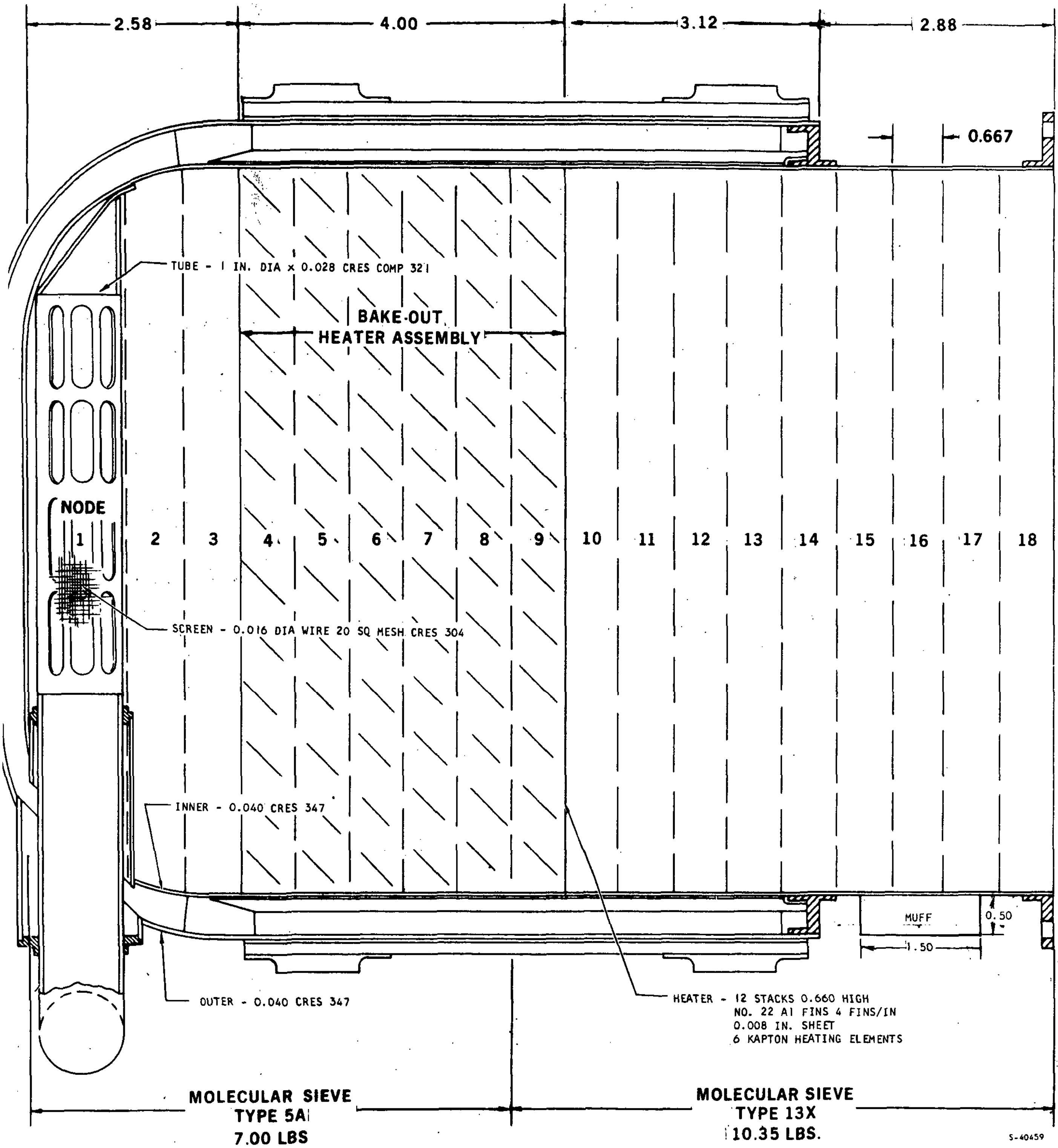

Figure 4-1. Molecular Sieve Canister for Airlock Application

$$HSG = Nu \times k/d = 8.2 \times 0.01475/0.00603 = 20$$

During desorption, the thermal conductivity of the gas drops to 0.0022 Btu/hr ft ^{0}F, (Reference 5). Thus, HSG becomes

$$HSG = 8.2 \times 0.0022/0.00603 = 3.0$$

2. Sorbent to Shell

The term HXS accounts for all heat exchange between the sorbent and the canister wall. To make these calculations, the effective thermal conductivity of the sorbent must be known. (This is also necessary for the term SK.) Phillips (Reference 6) has obtained a correlation for bed thermal conductivity as a function of the gas conditions as well as the sorbent.

For the conditions here during adsorption:

SK = 0.10 Btu/(sq ft)(hr)(^{0}F/ft)

and for desorption, } bulk pack

SK = 0.08 Btu/(sq ft)(hr)(^{0}F/ft)

The conductivity in the heater section is then estimated by using volume weighted average of heater and sorbent conductivities. During adsorption,

SK = 11.6

and during desorption, } heat exchanger

SK = 11.6

The heat transfer coefficients are found by assuming a conductance path. In the bulk pack sections the path is taken as one-half the distance from the canister wall to the center of the bed. This yields a coefficient during adsorption of,

$$HXS = k/\Delta X = 0.10/0.145 = 0.685$$

during desorption,

$$HXS = 0.08/0.145 = 0.55$$

In the heat exchanger core the same conductance path was used. However, the mixed Al-MS conductivity is used. During adsorption the coefficient becomes

$$HXS = 11.6/0.146 = 79.5$$

during desorption, the coefficient is

$$HXS = 11.6/0.146 = 79.5$$

3. Gas to Shell

The gas to shell heat exchange accounts for a very small portion of the total energy transfer. The coefficient is calculated throughout the canister as the conductivity divided by the average heat path.

$$HXG = 0.01475/0.146 = 0.101$$

during desorption

$$HXG = 0.0022/0.146 = 0.0151$$

Diffusion Coefficients for CO_2 in 5A and H_2O in 13X

DIF = 4.0×10^{-4} throughout. No internal mass transfer resistance results from the use of this size diffusion coefficient.

Mass-Transfer Coefficients

The following mass transfer coefficients are determined from test data obtained at AiResearch.

1. Adsorption

$$GK_{CO_2} - 5A = 0.9 \times 10^{-4}$$

$$GK_{H_2O} - 13_X = 5.0 \times 10^{-3}$$

2. Desorption

$$GK_{CO_2} - 5A = 5.0 \times 10^{-4}$$

$$GK_{H_2O} - 13_X = 1.0 \times 10^{-3}$$

Properties of Sorbents

1. Sorbent Density

RHØS = 64 lb/cu ft

2. Bulk Density

RHØSB = 45 lb/cu ft in bulk pack

RHØSB = 36 lb/cu ft in heater core

Heat of Adsorption

The following heat of adsorption data are calculated from equilibrium isotherm data as described in (Reference 7).

DH = 400 for CO_2 on 5A (Btu/lb)

DH = 1400 for H_2O on 13X (Btu/lb)

Equilibrium Data

Equilibrium data for H_2O - 13X and CO_2 -5A are fitted by equations and are used in FUNCTION PKEQ.

Vacuum Duct and Gas Valve Characteristics

The gas discharge capacity of the vacuum duct with gas valve for the Airlock molecular sieve system was found to be approximated by the following expression:

$$W_D\ (P) = \left[\ell n \left(\frac{P}{0.888} \right) + 1.76 \right] / 1.96 \qquad (4-1)$$

This equation is used in subroutine DESORB for the present simulation.

SUMMARY AND LISTING OF INPUT DATA

Summary of Input Data

A summary of the input data for the example problem is presented in Figure 4-2.

Listings of the input and output data are given in the following pages.

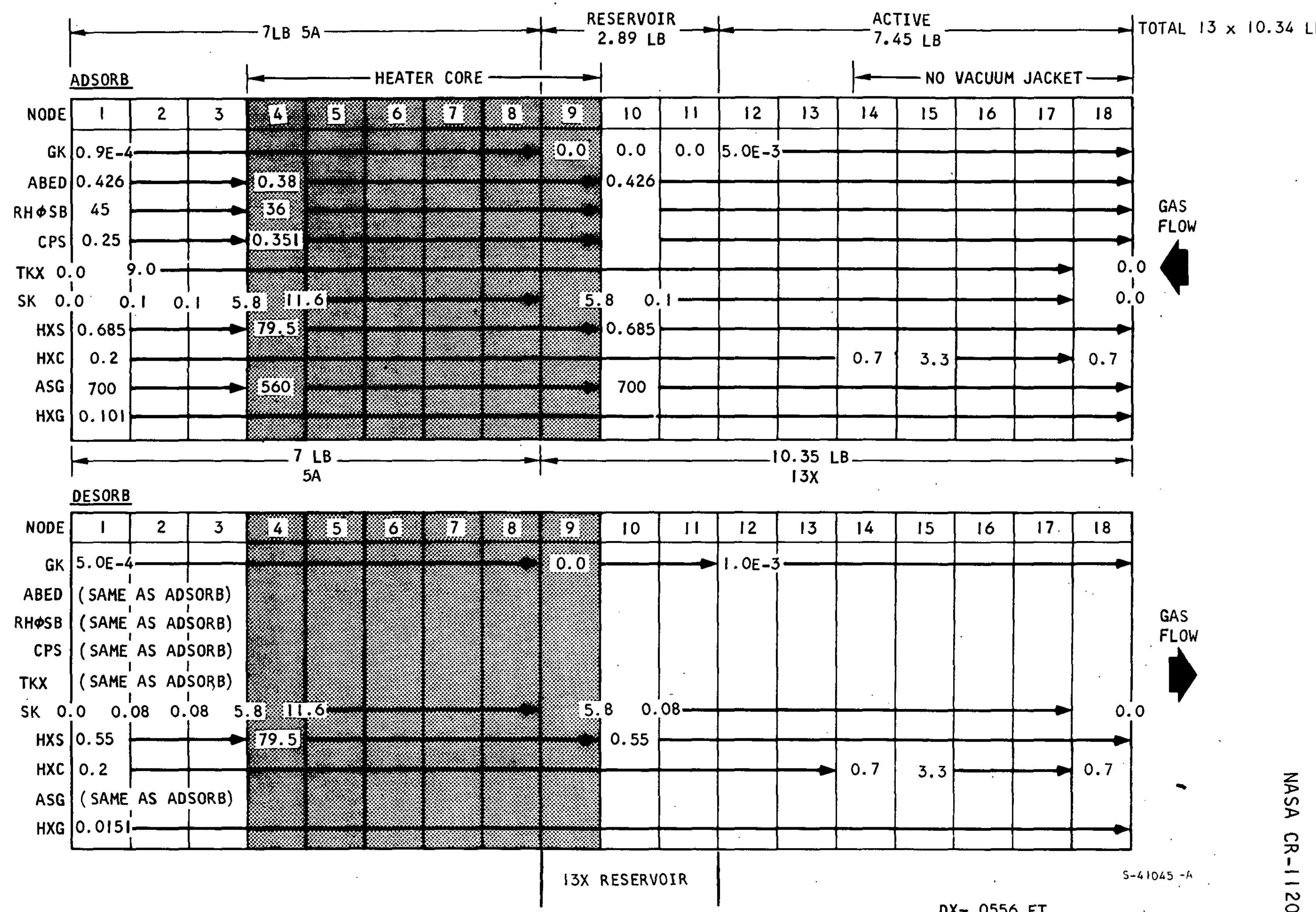

Figure 4-2. Computer Nodal Parameters For Air-Lock CO_2 Removal System

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INPUT DATA FOR EXAMPLE PROBLEM

```
@ ELT S9973,1,690617, 53904     ,1
      BLOCK DATA
C  INPUT DATA TO ADSORB
      COMMON /BLOK2/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK6/ NCYCLT
      COMMON/BLOK10/ NPRINT,DTMAX,NDTCON
      COMMON /BLOK12/ NTEMP
      COMMON /BLOK13/ WI, TI
      COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RCO2C
      COMMON /BLOK17/ NSTART
      DIMENSION AXS(41),AXG(41),AGS(41),HSX(41),HGX(41),HGS(41),ACX(41),
     1HCX(41)
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS),(AXC,ACX),(HXC,HCX)
C
C  BED CONFIGURATION
C
      DATA ABED/3*.426,6*.38,9*.426,23*0./
      DATA NDX1, NDXM, NDXMAC, NDR4, DX  / 18, 11, 8, 2, 0.0556/
      DATA AGX  / 41*6.18/
      DATA ASX  / 41*6.18/
C  SORBENT PROPERTIES
C  SORBENT PROPERTIES
C
      DATA ASG/3*700.,6*560.,9*700.,23*0.0/
      DATA CPS/3*.25,6*.351,9*.25,23*0.0/
      DATA RHOS /64., 64. /
      DATA RHOSB/3*45.,6*36.,9*45.,23*0.0/
      DATA SK/0.0,2*.1,5.8,5*11.6,5.8,8*.1,23*0.0/
C  COOLANT PROPERTIES
C
      DATA AVC  / 41*100. /
      DATA CPC/41*1.E20/
      DATA NOG  / 1 /
      DATA T268 /70./
      DATA UC/41*0.0/
C  HEAT TRANSFER COEFFICIENTS
C
      DATA HSG  / 41*20.  /
      DATA HXC/13*0.2,.7,3*3.3,.7,23*0.0/
      DATA HXG/18*0.101,23*0.0/
      DATA HXS/3*.685,6*79.5,9*.685,23*0.0/
C  INITIAL CONDITIONS
C
      DATA TC/14*70.,3*65.,24*70.0/
      DATA TG/8*55.,3*75.,3*80.,75.,60.,40.,23.,23*50./
      DATA TS/8*55.,3*75.,3*80.,75.,60.,40.,23.,23*50./
      DATA TX/41*70./
```

```
      DATA W/168*.03100,63*1.D-3,21*.1200,21*.13700,21*.1500,21*.16D0,
     121*.1800,21*.200,21*.20500,483*1.D-3/
C  MASS TRANSFER PROPERTIES
C
      DATA DIF/41*4.E-4/
      DATA GK   /8*0.9E-4, 3*0.0, 7*5.E-3, 23*0.0 /
C  PROCESS GAS STREAM PROPERTIES
C
      DATA CPG  / 41*0.23 /
      DATA DH   / 11*400., 7*1400.,  23*0.0 /
      DATA WM   / 44.0, 18.0 /
C  HXCORE PROPERTIES
      DATA AVX  /41*375./
      DATA CPX  / 41*0.11/
      DATA RHOX/ 41*490./
      DATA TKX  / 0., 17*9.0,23*0.0/
C  MISCELLANEOUS CONTROL PARAMETERS
C
      DATA CYCLE/ 0.25/
      DATA NTEMP/ 1/
      DATA NCYCLT,NSTART/10,10/
      DATA NPRINT/10/
      DATA WI,TI/ 0.005, 1.5 /
      DATA DTMAX/ 0.005 /
      DATA NDTCON/ 1 /
C  ADSORB PARAMETERS
C
      DATA PCO2C, PH2OI, TGI /7.0, 10., 52. /
      DATA VOLCAB, RCO2C / 320.0, 0.281 /
      DATA GMR,GMW/10.,28.04/
      DATA PA/258./
      END
```

```
@ ELT S9993,1,690617, 53905    ,1
      BLOCK DATA
C  INPUT DATA TO DESORB
      COMMON /BLOK1/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      DOUBLE PRECISION C1P,C2P,C3P,D1P
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
     1         CP1,CP2,X,DT
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK4/ POUT(10),TIMET(10),NBCOUT,NPSET(3)
      COMMON /BLOK6/ NCYCLT
      COMMON /BLOK10/ NPRINT,DTMAX,NDTCON
      COMMON /BLOK12/ NTEMP
      COMMON /BLOK13/ WI, TI
      COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RCO2C
      COMMON /BLOK17/ NSTART
      DIMENSION AXS(41),AXG(41),AGS(41),HSX(41),HGX(41),HGS(41),ACX(41),
     1HCX(41)
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS),(AXC,ACX),(HXC,HCX)
C  BED CONFIGURATION
C
      DATA ABED/3*.426,6*.38,9*.426,23*0./
      DATA NDX1, NDXM, NDXMAC, NDR4, DX / 18, 11, 8, 2, 0.0556/
      DATA AGX  / 41*6.18/
      DATA ASX  / 41*6.18/
C  SORBENT PROPERTIES
C
      DATA ASG/3*700.,6*560.,9*700.,23*0.0/
      DATA CPS/3*.25,6*.351,9*.25,23*0.0/
      DATA RHOS /64., 64. /
      DATA RHOSB/3*45.,6*36.,9*45.,23*0.0/
      DATA SK/0.0,2*.08,5.8,5*11.6,5.8,8*.08,23*0.0/
C  COOLANT PROPERTIES
C
      DATA AVC  / 41*100. /
      DATA CPC/41*1.E20/
      DATA NOG  / 1 /
      DATA T268 /70./
      DATA UC/41*0.0/
C  HEAT TRANSFER COEFFICIENTS
C
      DATA  HSG /41*3.0 /
      DATA HXC/13*0.2,.7,3*3.3,.7,23*0.0/
      DATA HXG/18*0.0151,23*0.0/
      DATA HXS/3*0.55,6*79.5,9*.55,23*0.0/
C  MASS TRANSFER PROPERTIES
C
      DATA DIF/41*4.E-4/
      DATA GK/8*5.E-4,3*0.0,7*1.E-3,23*0.0/
```

```
C  PROCESS GAS STREAM PROPERTIES
C
      DATA CPG   / 41*0.23 /
      DATA DH   / 11*400., 7*1400.,  23*0.0 /
      DATA WM    / 44.0, 18.0 /
C  HXCORE PROPERTIES
C
      DATA AVX   / 41*375./
      DATA CPX   / 41*0.11/
      DATA RHOX/ 41*490./
      DATA TKX   / 0., 17*9.0,23*0.0/
C  DESORB PARAMETERS
C
      DATA NBCOUT/ 1/
      DATA NPSET / 0,0, 18/
      END
```

```
@ ELT S9992,1,690501, 43774
      FUNCTION PKEQ(ID,W,T)
C     PKEQ=EQUILIBRIUM PRESSURE IN MM HG
C     ID=2,H2O ON 13X
C     ID=1,CO2 ON MOLECULAR SIEVE 5A
C     W=LOADING IN LB ADSORBATE PER LB ADSORBENT
C     T=TEMP IN DEG F
      DATA B1/.0705230784 /
      DATA B2/.0422820123 /
      DATA B3/.0092705272 /
      DATA B4/.0001520143 /
      DATA B5/.0002765672/
      DATA B6/.0000430638/
C
      IF (W .LE. 0. ) W= 1.E-5
      GO TO (41,51),ID
   41 CONTINUE
      Y=ALOG(W)
      YBIG=0.667*Y+2.22+0.0025*T
      H=ABS(YBIG)
      IF (H .GE. 1.0) GO TO 231
      IF(H-.0001) 15,15,16
   15 XBIG=1.7725*H/2.0
      GO TO 18
   16 CONTINUE
      IF(H .LE. 0.84) GO TO 1
      IF(H .LE. 0.88) GO TO 2
      IF (H .LE.  0.934) GO TO 3
      IF (H .LE.  0.984) GO TO 8
      IF (H .LE.  0.997) GO TO 5
      X0=2.2+200.*(H-0.998)
      GO TO 6
  231 H=1.0
      GO TO 17
    1 X0=H
      GO TO 6
    2 X0=1.0
      GO TO 6
    3 X0=1.2
      GO TO 6
    8 X0=1.3+8.*(H-.934)
      GO TO 6
    5 X0=1.7+30.*(H-.984)
    6 HPRX0=(2./1.77245)*EXP(-1.*(X0)**2)
      C=-16.
      HNEW=1.+X0*(B1+X0*(B2+X0*(B3+X0*(B4+X0*(B5+X0*(B6))))))
      HNEW=1.-HNEW**C
      DELH=H-HNEW
      TERM=DELH/HPRX0
      XBIG=X0+TERM+X0*TERM**2+((4.*X0**2+1.)*TERM**3)/3.+(7.*X0+12.
     1*X0**3)*TERM**4/6.
      GO TO 18
   17 XBIG=4.0
   18 XBIG=SIGN(XBIG,YBIG)
   12 X=(XBIG-0.493+0.00953*T)/0.38
      PKEQ=EXP(X)
      RETURN
   51 CONTINUE
      PKEQ=EXP(47.2*W-1.31E4/(T+460.)+15.2)
```

RETURN
END

000059
000060

OUTPUT DATA FOR EXAMPLE PROBLEM

TOTAL VOLUME OF M.S. BED = .2452 CU FT
TOTAL WT OF M.S. BED = 9.893 LB
TOTAL VOLUME OF S.G. BED = .1658 CU FT
TOTAL WT OF S.G. BED = 7.461 LB
TOTAL WT OF ACTIVE M.S. BED = 7.001 LB

ADSORPTION CYCLE 3
TIME= .25000 HR 15.000 MIN TIME INCREMENT= .00010 HR

AXIAL NODE	PCO2,MM	PH20,MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	2.9659	.0266	73.5514	73.5399	69.9999	72.4927
2	3.3260	.0266	75.2208	75.2119	69.9999	73.1577
3	3.7410	.0266	76.5122	76.5127	69.9999	74.3898
4	4.2411	.0266	76.4586	76.4590	69.9999	76.2045
5	4.7296	.0266	76.4202	76.4211	69.9999	76.3174
6	5.3051	.0266	76.3211	76.3228	69.9999	76.2339
7	5.9265	.0266	76.1422	76.1446	69.9999	76.0612
8	6.5029	.0266	75.8939	75.8965	69.9999	75.8128
9	6.8842	.0266	75.6331	75.6358	69.9999	75.4556
10	6.8842	.0266	75.3529	75.3643	69.9999	73.9867
11	6.8842	.0266	73.7137	73.7079	69.9999	73.0152
12	6.8842	.0266	74.5609	74.5223	69.9999	72.6148
13	6.8842	.0758	80.1246	79.9936	69.9999	72.8505
14	6.8842	.3435	99.0533	98.8847	69.9999	73.5828
15	6.8842	2.2727	123.5266	123.5668	64.9999	73.3740
16	6.8842	5.7285	118.0636	118.1930	64.9999	73.2868
17	6.8842	7.5100	99.6914	99.8366	64.9999	72.5691
18	6.8842	8.8361	78.9300	79.1171	69.9999	72.6581

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB NODE / AXIAL NODE	AVG	1	2	3	4	5	6	7	8	9	10	11
1	.0356	.0356	.0357									
2	.0369	.0369	.0370									
3	.0385	.0384	.0386									
4	.0408	.0407	.0409									
5	.0433	.0431	.0434									
6	.0466	.0464	.0467									
7	.0506	.0504	.0507									
8	.0551	.0550	.0552									
9	.0010	.0010	.0010									
10	.0010	.0010	.0010									
11	.0010	.0010	.0010									
12	.1198	.1198	.1198									
13	.1364	.1364	.1365									
14	.1507	.1505	.1508									
15	.1708	.1705	.1710									
16	.1948	.1946	.1949									
17	.2162	.2161	.2163									
18	.2388	.2387	.2388									

AVG CO2 LOADING IN M.S. BED = .0426 LB/LB AVG H20 LOADING IN S.G. BED = .1753 LB/LB

TIME AVG CO2 ADSORP RATE = .2769 LB/HR TIME AVG H20 ADSORP RATE = .2482 LB/HR

TIME AVG EXIT PH2O = .0261 MM

TIME AVG RATE OF M.S. POISONING BY H2O = .6495-03 LB H2O/HR

DESORPTION CYCLE 3
TIME= .25000 HR 15.000 MIN TIME INCREMENT= .00106 HR

AXIAL NODE	TOTAL PRESS,MM	GAS TEMP,DEG F	SORBENT TEMP, DEG F	COOLANT TEMP,DEG F	HX CORE TEMP, DEG F
1	1.7978	67.4260	67.4260	69.9999	68.3718
2	1.7859	66.5355	66.5353	69.9999	67.8291
3	1.7621	64.9264	64.9259	69.9999	66.7709
4	1.7261	65.0595	65.0596	69.9999	65.2339
5	1.6854	65.1453	65.1454	69.9999	65.1883
6	1.6349	65.2648	65.2649	69.9999	65.2970
7	1.5744	65.4216	65.4218	69.9999	65.4533
8	1.5036	65.6162	65.6164	69.9999	65.6568
9	1.4224	65.8453	65.8456	69.9999	66.0016
10	1.3297	66.0852	66.0854	69.9999	67.6673
11	1.2186	72.1368	72.1426	69.9999	68.9369
12	1.1049	73.9355	73.9373	69.9999	69.5487
13	.9872	76.6363	76.6392	69.9999	69.4571
14	.8639	78.0037	78.0054	69.9999	68.4589
15	.7324	70.9618	70.9550	64.9999	66.2688
16	.5901	54.5498	54.5321	64.9999	63.9891
17	.4336	34.8350	34.8117	64.9999	61.7366
18	.2574	15.6726	15.6465	69.9999	59.7257

AXIAL NODE	MOLE FRAC	CO2 RATE,M/HR	H2O RATE,M/HR
1	1.000000	.000526	.000000
2	1.000000	.001054	.000000
3	1.000000	.001795	.000000
4	1.000000	.002332	.000000
5	1.000000	.002876	.000000
6	1.000000	.003426	.000000
7	1.000000	.003978	.000000
8	1.000000	.004521	.000000
9	1.000000	.004521	.000000
10	1.000000	.004521	.000000
11	1.000000	.004521	.000000
12	.017900	.004521	.000083
13	.051202	.004521	.000243
14	.111674	.004521	.000562
15	.191927	.004521	.001062
16	.274719	.004521	.001702
17	.345515	.004521	.002380
18	.426412	.004521	.003358

LOADING AT INTERIOR OF SORBENT

SORB NODE / AXIAL NODE	AVG	1	2	3	4	5	6	7	8	9	10	11
1	.0323	.0323	.0322									
2	.0327	.0328	.0326									
3	.0338	.0339	.0337									
4	.0333	.0334	.0332									
5	.0328	.0329	.0327									

6	.0322	.0322	.0321
7	.0313	.0314	.0312
8	.0303	.0304	.0302
9	.0010	.0010	.0010
10	.0010	.0010	.0010
11	.0010	.0010	.0010
12	.1194	.1194	.1194
13	.1356	.1356	.1356
14	.1482	.1482	.1481
15	.1633	.1633	.1632
16	.1834	.1834	.1833
17	.2038	.2038	.2037
18	.2238	.2238	.2237

AVG CO2 LOADING IN M.S. BED = .0324 LB/LB   AVG H2O LOADING IN S.G. BED = .1682 LB/LB

TIME AVG CO2 DESORP RATE = .2843 LB/HR   TIME AVG H2O DESORP RATE = .2135 LB/HR

SECTION 5

REFERENCE INFORMATION

SUBPROGRAM DOCUMENTATION

Main Program (S9950)

This main program calls MADSOR to perform one adsorption half-cycle calculation.

Main Program (S9951)

This main program calls MDESOR to carry out one desorption half-cycle calculation.

MADSOR (S9970)

This subroutine monitors the adsorption half-cycle calculations. It prints the total quantities of molecular sieve and silica gel pellets in the composite bed for input data check-out purposes. The routine, then, calls STARTA. The time increment size for the next time step is selected such that TI and WI specified in the input data are satisfied. Subroutine ADSORB is then called to advance one time step, new cabin P_{CO_2} is calculated and the results are printed if this should be done according to NPRINT, and NSTART.

The program flow chart is given in Figure 5-1.

STARTA (S9978)

Everything which stays constant throughout the entire adsorption half cycle is evaluated in this subroutine. A, RS, CR1, CR2, CR3 are evaluated in the subroutine.

ADSORB (S9971)

This subprogram computes all the coefficients required in Equations (2-64) through (2-69), solve for p_k's first, followed by bed loadings, and temperatures. A logic diagram of the subprogram is shown in Figure 5-2.

TSØRBA (S9977)

This routine solves Equation (2-32) for adsorption period sorbent temperatures, using the method shown in Equations (2-38) through (2-46).

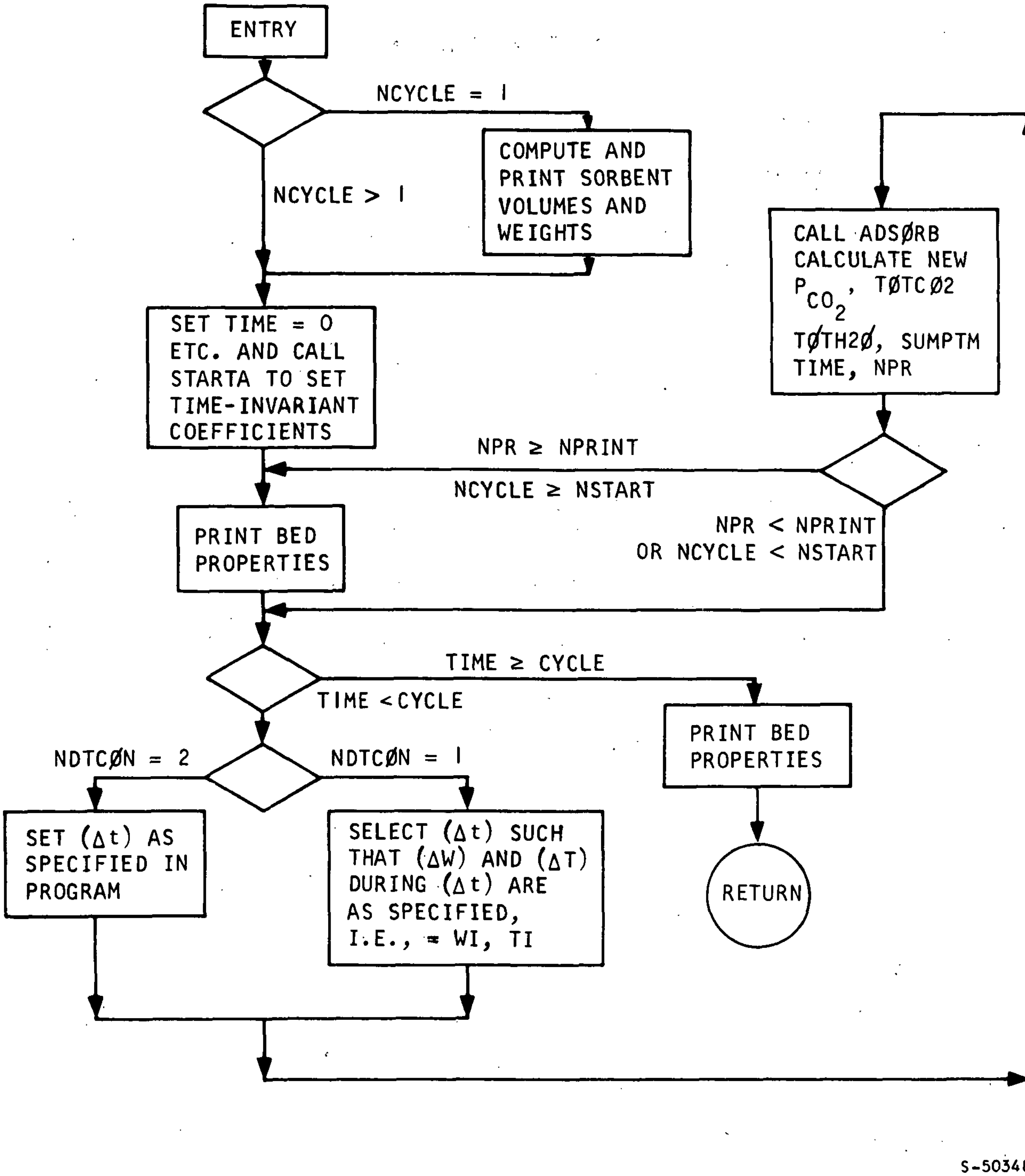

Figure 5-1. Logic Flow Chart for MADSOR

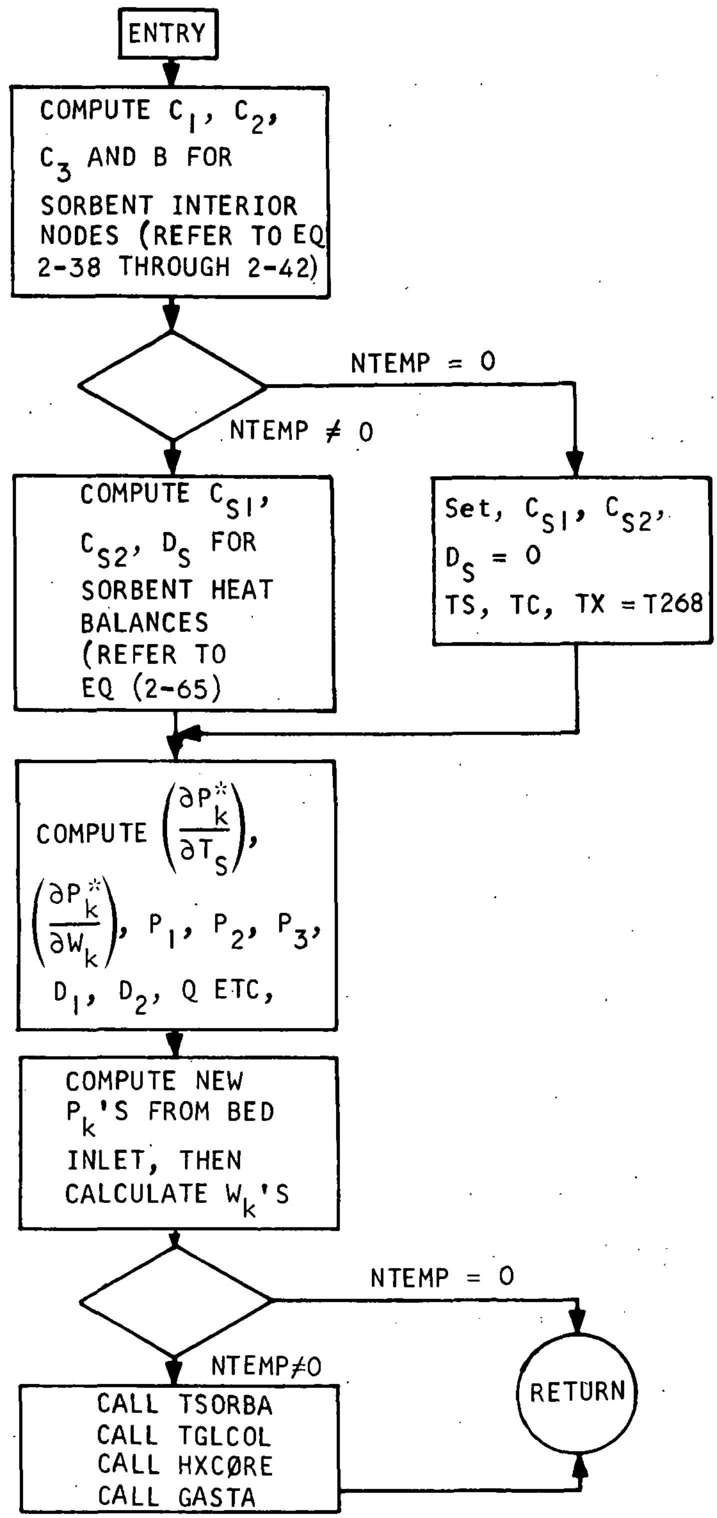

Figure 5-2. Logic Flow Chart for ADSORB

TGLCØL (S9987)

Equation (2-33) is solved for coolant temperatures using the method described by Equations (2-38) through (2-46).

HXCØRE (S9991)

Equation (2-34) is solved for heat exchanger core temperatures using the method described in Equations (2-38) through (2-46).

GASTA (S9976)

Equation (2-31) is used to obtain gas temperatures for the adsorption period. Arguments of the subroutine are

CMR = process gas flow rate, lb/hr

CPG = specific heat of process gas stream, Btu/(lb)(^{o}F)

ABED = cross-sectional area, (sq ft)

NDXI = total number of axial nodes

TGI = process gas inlet temperature, ^{o}F

ASG = sorbent surface area per unit bulk volume, (sq ft)/(cu ft)

HSG = heat transfer coefficient between gas and sorbent, Btu/(sq ft) (hr) (^{o}F)

AXG = primary heat transfer area between heat exchanger and gas, (sq ft)/(cu ft)

HXG = heat transfer coefficient between heat exchanger and gas, Btu/(hr)(sq ft) (^{o}F)

DX = axial increment size, ft

TG = gas temperature, ^{o}F

TS = sorbent temperature, ^{o}F

TX = heat exchanger temperature, ^{o}F

PRADSB (S9979)

This is the print routine for the adsorption program. A detailed description of output variables was given in Section 3.

MDESOR (S9980)

The routine controls desorption calculations much as MADSOR does the adsorption counterpart. It calls START, picks up a Δt, calls DESORB, PRDESB, and stores temperatures.

START (S9988)

Similar to STARTA for the adsorption, this subroutine generates all the coefficients which stay unchanged for the entire desorption half cycle.

PRDESB (S9989)

This is a print routine for the desorption program. For a detailed description of output variables, refer to Section 3.

DESØRB (S9983)

Heat and material balance equations for the desorption period are solved by the method described in Section 2. The coefficients required in Equations (2-48) through (2-62) are computed, the desorption pressure Equation (2-58) is solved in double precision and these pressures are used to calculate new bed loadings and temperatures. A logic flow chart for this subprogram is given in Figure 5-3.

TSØRB (S9997)

This routine solves for sorbent temperature in the desorption period, using the method described by Equations (2-38) through (2-46).

GAST (S9986)

The routine solves Equation (2-31) for the desorption period gas temperatures. Arguments of the subprogram are defined:

DX = axial increment size, ft

RHØG = density of vapor mixture, lb/(cu ft)

CPG = specific heat of vapor mixture, Btu/(lb)(^{o}F)

U = linear velocity of vapor mixture, ft/hr

TS = sorbent temperature, ^{o}F

TX = heat exchanger temperature, ^{o}F

NDXI = total number of axial nodes

ASG = sorbent surface area per unit bulk volume, (sq ft)/(cu ft)

HSG = heat transfer coefficient between gas and sorbent, Btu/(hr)(sq ft)(^{o}F)

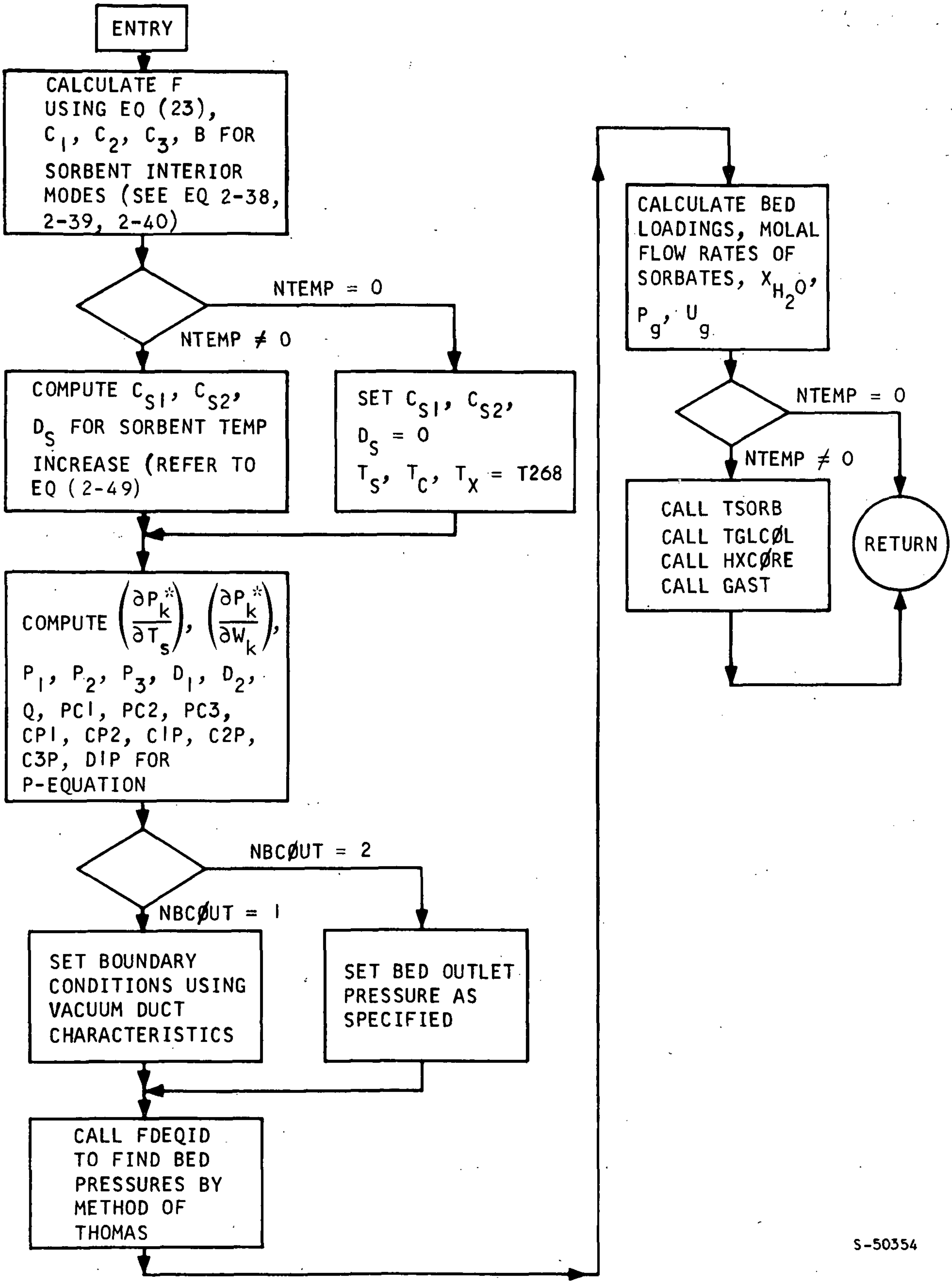

Figure 5-3. Logic Flow Chart for DESORB

AXG = primary heat transfer area between heat exchanger and gas, (sq ft)/(cu ft)

HXG = heat transfer coefficient between heat exchanger and gas, Btu/(hr)(sq ft)(^{0}F)

TG = gas temperature, ^{0}F

VØIDF = void fraction

PKEQ (S9992)

This function subprogram calculates the equilibrium CO_2 and H_2O vapor pressures over the molecular sieve and desiccant sorbents, respectively.

Arguments of the function are

ID = control index, ID = 1 indicates CO_2 over molecular sieve sorbent, ID = 2 indicates H_2O over desiccant sorbent.

W = loading, lb-sorbate/(lb-sorbent)

T = sorbent temperature, ^{0}F

IFN (S9981)

The function determines whether a given axial node belongs in the molecular sieve bed or desiccant bed.

FDEQIM (S9984)

The routine solves a system of finite difference equations by the method described by Equations (2-38) through (2-46).

FDEQID (S9985)

The subroutine is a double precision version of FDEQIM.

LAGIN2 (S9996)

This routine performs a Lagrangian polynomial interpolation. Arguments variables are:

ID = in case of trouble, this ID number will be printed for program checkout

X = independent variable

NP = number of tabulated pairs of data to be used

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Los Angeles, California

ND = Number of points to be used in interpolation. For instance if ND = 2, linear interpolation will be used

XØ = value of independent variable X

YØ = value of dependent variable corresponding to XØ (this is the answer obtained by LAGIN2)

Y = dependent variable

SOURCE PROGRAM LISTING

AIRESEARCH MANUFACTURING COMPANY
Los Angeles, California

```
@ ELT S9960,1,690501, 43778
C      MAIN PROGRAM FOR COMBINED ADSORPTION/DESORPTION PROGRAM -- DEVELOPED
C      BY K C HWANG, AIRESEARCH , LOS ANGELES
C
       COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
       DOUBLE PRECISION W
       COMMON /BLOK6/ NCYCLT
       COMMON /BLOK14/ NCYCLE
       NCYCLE=1
    11 CONTINUE
       WRITE (6,300)
       CALL MADSOR
       WRITE (6,400)
       CALL MDESCR
       NCYCLE=NCYCLE+1
       IF(NCYCLE .LE. NCYCLT) GO TO 11
       CALL EXIT
   300 FORMAT(24H1 START ADSORPTION CYCLE )
   400 FORMAT(24H1 START DESORPTION CYCLE )
       END
```


322321

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```
@ ELT S995D,1,690501, 43776
000001          CALL MADSOR
000002          END
```

```
@ ELT S9951,1,690501, 43777

000001              CALL MDESOR
000002              END
```

```
,@ ELT S9970,1,690501, 43780
      SUBROUTINE MADSOR
C
      COMMON /BLOK2/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      COMMON /BLOK10/ NPRINT,DTMAX,NDTCON
      COMMON /BLOK11/ TOTCO2,TOTH2O,SUMPTM,WTACMS,WTSG
      COMMON /BLOK13/ WI, TI
      COMMON /BLOK14/ NCYCLE
      COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RCO2C
      COMMON /BLOK17/ NSTART
C
      IF(NCYCLE .GT. 1) GO TO 1
      N1=NDXM+1
      VMS = 0.0
      WTMS=0.0
      VSG=0.0
      WTSG=0.0
      IF(NDXM .EQ. 0) GO TO 11
      DO 10 N= 1, NDXM
      VMS=VMS+DX*ABED(N)
      WTMS=WTMS+DX*ABED(N)*RHOSB(N)
   10 CONTINUE
   11 CONTINUE
      IF((NDX1-NDXM) .EQ. 0) GO TO 31
      DO 30 N= N1,NDX1
      VSG=VSG+DX*ABED(N)
      WTSG=WTSG+DX*ABED(N)*RHOSB(N)
   30 CONTINUE
   31 CONTINUE
      WRITE(6,500) VMS, WTMS, VSG, WTSG
  500 FORMAT(  28H1TOTAL VOLUME OF M.S. BED = G10.4,2X,5HCU FT//
     123H TOTAL WT OF M.S. BED =   G10.4,2X, 2HLB//
     228H TOTAL VOLUME OF S.G. BED =  G10.4,2X,5HCU FT//
     323H TOTAL WT OF S.G. BED =   G10.4, 2X,2HLB)
      WTACMS=0.0
      IF(NDXMAC .EQ. 0) GO TO 12
      DO 70 N= 1, NDXMAC
   70 WTACMS=WTACMS + DX*ABED(N)*RHOSB(N)
   12 CONTINUE
      WRITE(6,501) WTACMS
  501 FORMAT( /  30H TOTAL WT OF ACTIVE M.S. BED =  , G10.4,3H LB )
    1 TIME = 0.0
      SUMPTM=0.
      DT = 1.E-5
      DTO =0.0
      TOTCO2=0.0
      TOTH2O=0.0
```

```
      DO 20 N=1,NDX1
      TS1(N)= TS(N)
      TS2(N)= TS(N)
      TX1(N)=TX(N)
      TX2(N)=TX(N)
      TC1(N)=TC(N)
      TC2(N)=TC(N)
   20 CONTINUE
      CALL STARTA
      NPR=NPRINT - 1
      GO TO 3
    2 CALL PRADSB
      NPR = 0
    4 CONTINUE
      IF( TIME .GE. CYCLE) CALL PRADSB
      IF( TIME .GE. CYCLE) GO TO 9999
      DTO=DT
      GO TO (41,42),NDTCON
   41 ADT=DTMAX
      DO 60 N=1,NDX1
      ADT2=WI      /(ABS(W(NDR4,N)-WS(N))+1.E-9)*DT
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TS(N)-TS2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TX(N)-TX2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TC(N)-TC2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
   60 CONTINUE
      DT=ADT
      GO TO 3
   42 DT=DTMAX/10.0
      IF(TIME .GT. 0.06) DT=DTMAX
    3 CONTINUE
      IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
      DO 21 N=1,NDX1
      TS2(N)=TS1(N)
      TS1(N)=TS(N)
      TX2(N)=TX1(N)
      TX1(N)=TX(N)
      TC2(N)=TC1(N)
      TC1(N)=TC(N)
   21 CONTINUE
      PCO2I = PCO2C
      CALL ADSORB(DT)
      DPCO2C = DT*(RCO2C - GMR*
     1                         (PCO2I-PK(1,1))*44./(PA*GMW))*554.*530./(44.*
     2VOLCAB)
      PCO2C= PCO2C+DPCO2C
      TOTCO2=TOTCO2+GMR*DT*(PCO2I-PK(1,1))*44./(PA*GMW)
      TOTH2O=TOTH2O+GMR*DT*(PH2OI-PK(2,1))*18./(PA*GMW)
      SUMPTM= SUMPTM+PK(2,1)*DT
      TIME=TIME+DT
      NPR = NPR+1
      IF( (NPR.GE. NPRINT) .AND. (NCYCLE .GE. NSTART) ) GO TO 2
      GO TO 4
 9999 CONTINUE
      RETURN
      END
```

```
@ ELT S9971,1,690617, 53908   ,1
      SUBROUTINE ADSORB(DELT)
      COMMON /BLOK2/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      COMMON /BLOK12/ NTEMP
      DIMENSION AS(2)
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS)
      DT = DELT
      AS(1)=4.*3.1416*RS(1)**2
      AS(2)=4.*3.1416*RS(2)**2
C
C
C
      DATA RGAS/554./
C
      NDR=NDR4-1
      DO 21 N=1,NDX1
      I=IFN(N,NDXM)
      DO 20 NR=1,NDR4
      C1(NR,N)=-CR2(I,NR)
      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
   20 C3(NR,N)=-CR3(I,NR)
C
C
      B(1,N)=C3(1,N)/C2(1,N)
      DO 21 J=2,NDR
   21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
      NDX=NDX1-1
C     TO TEMPORARILY STORE SURFACE LOADING
      DO 50 N=1,NDX1
   50 WS(N)=W(NDR4,N)
      IF (NTEMP .EQ. 0 ) GO TO 111
C
C     TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
      DO 12 N=1,NDX1
      I=IFN(N,NDXM)
      CS2(N)=DT/CPS(N)/RHOSB(N)*ABG(N)*GK(N)*WM(I)*DH(N)
      CS1(N) = CS2(N)
      IF(N.EQ.1) S1=(
     1(ABED(N)+ABED(N+1))*SK(N+1)*(TS(N+1)-TS(N)))
     2/(2.*ABED(N)*DX*DX)
      IF(N.EQ. 1) GO TO 15
      S1=((ABED(N-1)+ABED(N))*SK(N)*(TS(N-1)-TS(N))+
     1(ABED(N)+ABED(N+1))*SK(N+1)*(TS(N+1)-TS(N)))
     2/(2.*ABED(N)*DX*DX)
   15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+
     1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
```

```
      RATIO = (DT+DTO)/DT
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=RATIO*CS1(N)/(1.+T1)
      CS2(N)=RATIO*CS2(N)/(1.+T1)
      DS(N)=RATIO*DS(N)
      DS(N)= (DS(N)-T1*TS2(N))/(1.+T1)
   12 CONTINUE
      GO TO 110
  111 DO 112 N= 1, NDX1
      CS1(N)=0.
      CS2(N)=0.
      DS(N)=0.
      TS(N)=T268
      TC(N)=T268
      TX(N)=T268
      TG(N)=T268
  112 CONTINUE
  110 CONTINUE
C
C     TO CALCULATE PARTIAL PRESSURE OF ADSORBATE IN GAS STREAM
C
      DO 24 N=1,NDX1
      I=IFN(N,NDXM)
C     TO CALCULATE P1,P2,P3
      WSURF=W(NDR4,N)
      PSURF= PKEQ(I,WSURF,TS2(N))                                              *NEW
      DPKDTS=                                                                  **-1
     1(PKEQ(I,WSURF,(TS2(N)+0.001))-PSURF)/                                    *NEW
     20.001                                                                    **-1
      DPKDWK=(PKEQ(I,(WSURF+1.E-6),TS2(N))-PSURF)/1                            *NEW
     1.E-6                                                                     **-1
      G=1.+CS2(N)*DPKDTS
      P1(N)=(PSURF                    +DS(N)*DPKDTS)/G
      P2(N)=DPKDWK/G
      P3(N)=CS1(N)/G*DPKDTS
C
      C2(NDR4,N)=CR1(I,NDR4)/DT+CR2(I,NDR4)+WM(I)*GK(N)*P2(N)*AS(I)
      C3(NDR4,N)=0.0
      DO 23 NR=1,NDR4
   23 D1(NR,N)=CR1(I,NR)/DT*W(NR,N)
      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(I)
      D2(N)=AS(I)*WM(I)*GK(N)*( 1.     -P3(N))
      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))
      Q(1,N)=D1(1,N)/C2(1,N)
      DO 24 J=2,NDR4
   24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
C
      DO 25 N=1,NDX1
      I=IFN(N,NDXM)
      CP1(N)=ASG(N)*GK(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
   25 CP2(N)=ASG(N)*GK(N)*(P2(N)*D2(N)+P3(N)-1.0)
      PK(1,NDX1+1) = PCO2I
      PK(2,NDX1+1) = PH2OI
      DO 26 N=1,NDX1
      N1=NDX1+1-N
      I=IFN(N1,NDXM)
      PK(I,N1) = (PK(I,N1+1)/DX+CP1(N1)/A(N1))
     1                                    /(1./DX-CP2(N1)/A(N1))
      IF (I.EQ.1)J=2
```

```
      IF(I.EQ.2)J=1
      PK(J,N1)=PK(J,N1+1)
   26 CONTINUE
C
C
C
C     TO CALCULATE SORBENT LOADING
C
      DO 30 N=1,NDX1
      I=IFN(N,NDXM)
      W(NDR4,N)=Q(NDR4,N)+D2(N)*PK(I,N)
      DO 30 J=2,NDR4
      L=NDR4+1-J
   30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
C
C
      IF( NTEMP .EQ. 0) RETURN
C     TO CALCULATE SORBENT,GLYCOL,HX CORE AND GAS TEMPERATURES
C
      CALL TSORBA
      CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,AVC,NOG)
      CALL HXCORE(TX,TC,TS,TG,HXC,HXS,HXG,RHOX,CPX,TKX,DX,DT,NDX1,AVX,
     1NDXM)
      CALL GASTA(GMR,CPG,ABED,NDX1,TGI,ASG,HSG,AXG,HXG,DX,TG,TS,TX)
      RETURN
      END
```

```
* ELT S9976,1,690581, 43783
      SUBROUTINE GASTA(GMR,CPG,ABED,NDX1,TGI,ASG,HSG,AXG,HXG,DX,TG,TS,TX
     1)
C
C     GAS TEMPERATURE CALCULATIONS FOR ADSORPTION
C
      DIMENSION CPG(1),ASG(1),HSG(1),HXG(1),TG(1),TS(1),TX(1),ABED(1),
     1AXG(1)
C
      TG(NDX1+1) = TGI
      DO 10 N=1,NDX1
      N1=NDX1+1-N
      C=GMR*CPG(N1)/ABED(N1)
      C1=ASG(N1)*HSG(N1)+AXG(N1)*HXG(N1)
   10 TG(N1) = (TG(N1+1)/DX+(ASG(N1)*HSG(N1)*TS(N1)+AXG(N1)
     1                                          *HXG(N1)*TX(N1))/
     1C)/(1./DX+C1/C)
      RETURN
      END
```

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```
@ ELT 99977,1,690501, 43784

      SUBROUTINE TSORBA
      COMMON /BLOK2/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOC,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      DIMENSION S1(41),S2(41),S3(41),B1(41)
      DO 10 N=1,NDX1
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=CS1(N)*(1.0+T1)
      CS2(N)=CS2(N)*(1.0+T1)
      I=IFN(N,NDXM)
      TGAVG1=TG(N)
      B1(N) =TS2(N)*CS1(N)*
     1PK(I,N)
     2                          *CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)*WS(N))+
     1P3(N)*
     2PK(I,N)
     3              )+T*(ASG(N)*HSG(N)*TGAVG1+
     4ASX(N)*HXS(N)*TX1(N))-T1*TS2(N)
      IF(N.EQ.1) S1(N)=0.0
      IF(N.EQ.1) GO TO 11
      S1(N)=-T*SK(N)/DX/DX*(ABED(N-1)+ABED(N))/(2.*ABED(N))
   11 S3(N)=-T*SK(N+1)/DX/DX*(ABED(N)+ABED(N+1))/(2.*ABED(N))
      S2(N)=1.-S1(N)-S3(N)+T1
   10 CONTINUE
      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1)
      RETURN
      END
```

```
@ ELT S9978,1,690501, 43786
          SUBROUTINE STARTA
C
          COMMON /BLOK2/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
         1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
         2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,RS(41),RHOSB(41),DS(41),
         3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
         41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
         5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
         6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
         7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
         8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
         9,NDG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
          COMMON /BLOK3/ W(21,41),TC(41),TS(41),TC(41),TX(41),CYCLE
          DOUBLE PRECISION W
          DO 115 N=1,NDX1
      115 A(N)= GMR/ABED(N)/PA/GMW
C
C
          RS(1)=RHOSB(1)*3./RHOS(1)/ASG(1)
          RS(2)=RHOSB(NDX1)
         1           *3./RHOS(2)/ASG(NDX1)
          NDR=NDR4-1
          NDR2=2.*NDR
          NDR3=NDR2+1
          DO 10 I=1,2
          VS(I)=4./3.*3.1416*RS(I)**3
          DVS(I)=VS(I)/NDR
          DVS1(I)=DVS(I)/2
          RS1(I,1)=0.
          DO 10 K=2,NDR3
       10 RS1(I,K)=CBRT(3./4./3.1416*(4./3.*3.1416*RS1(I,K-1)**3+DVS1(I)))
          DO 11 I=1,2
          IF(I.EQ.1) DIF1=DIF(1)
          IF (I.EQ. 2) DIF1=DIF(NDX1)
          CR1(I,1)=DVS1(I)*RHOS(I)
          CR2(I,1)=0.
          CR3(I,1)=4.*3.1416*RS1(I,2)**2*DIF1  /(RS1(I,3)-RS1(I,1))*RHOS(I)
          DO 11 K=2,NDR4
          CR1(I,K)=DVS(I)*RHOS(I)
          CR2(I,K)=4.*3.1416*RS1(I,2*K-2)**2*DIF1  /(RS1(I,2*K-1)-RS1(I,2*K-
         13))*RHOS(I)
       11 CR3(I,K)=4.*3.1416*RS1(I,2*K)**2*DIF1  /(RS1(I,2*K+1)-RS1(I,2*K-1)
         1)*RHOS(I)
          CR1(1,NDR4)=CR1(1,1)
          CR1(2,NDR4)=CR1(2,1)
          RETURN
          END
```

```
@ ELT S9979,1,690901, 43767
      SUBROUTINE PRADSB
C
C
      DIMENSION AVLD(41)
      COMMON /BLOK2/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK4/ POUT(10),TIMET(10),NBCOUT,NPSET(3)
      COMMON /BLOK6/ NCYCLT
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      COMMON/BLOK10/ NPRINT,DTMAX,NDTCON
      COMMON /BLOK11/ TOTCO2,TOTH2O,SUMPTM,WTACMS,WTSG
      COMMON /BLOK12/ NTEMP
      COMMON /BLOK13/ WI, TI
      COMMON /BLOK14/ NCYCLE
      COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RCO2C
      COMMON /BLOK17/ NSTART
      DIMENSION AXS(41),AXG(41),AGS(41),HSX(41),HGX(41),HGS(41),ACX(41),
     1HCX(41)
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS),(AXC,ACX),(HXC,HCX)
      EQUIVALENCE(NDX,NDX1)
      AVPH2O = SUMPTM/TIME
      AVH2OP=GMR*AVPH2O*18./(PA*GMW)
C
      TIMEM=60.*TIME
      WRITE (6,100) NCYCLE, TIME, TIMEM, DT
      WRITE (6,101)
      WRITE(6,102)(N,PK(1,N),PK(2,N),
     1                    TG(N),TS(N),TC(N),TX(N),N=1,NDX)
      WRITE (6,202)
      N1=NDXM+1
      NDR3=NDR4-1
      DO 20 N= 1, NDXM
      SUMMS=0.0
      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
      IF(NDR4.EQ.2) AVLD(N) = SUMMS
      IF(NDR4.EQ.2) GO TO 20
      DO 22 NR=2,NDR3
   22 SUMMS=SUMMS+W(NR,N)
      AVLD(N)=SUMMS/NDR3
   20 CONTINUE
      DO 30 N= N1,NDX1
      SUMMS=0.0
      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
      IF(NDR4.EQ.2) AVLD(N) = SUMMS
      IF(NDR4.EQ.2) GO TO 30
      DO 33 NR=2, NDR3
   33 SUMMS=SUMMS+W(NR,N)
```

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```
      AVLD(N)=SUMMS/NDR3
   30 CONTINUE
      SUM=0.
      IF(NDXMAC .EQ. 0) GO TO 35
      DO 31 N= 1, NDXMAC
   31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVMSLD = SUM/WTACMS
      SUM=0.
   35 CONTINUE
      IF((NDX1-NDXM) .EQ. 0) GO TO 40
      DO 32 N= N1,NDX1
   32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVSGLD=SUM/WTSG
   40 CONTINUE
      DO 10 N=1,NDX
   10 WRITE (6,203)N, AVLD(N)
     1             ,(W(NR,N),NR=1,NDR4)
      WRITE (6,205) AVMSLD, AVSGLD
      AVRCO2=TOTCO2/TIME
      AVRH2O=TOTH2O/TIME
      WRITE(6,204) AVRCO2,AVRH2O
      WRITE(6, 206) AVPH2O, AVH2OP
      RETURN
  100 FORMAT (1H1,16HADSORPTION CYCLE  I3/
     1        3X,5HTIME=,F9.5,1X2HHR,F12.3,1X,3HMIN,
     1                                 5X,15HTIME INCREMENT=F7.5,1X2HHR)
  101 FORMAT (//2X,10HAXIAL NODE,3X,7HPCO2,MM,5X,7HPH2O,MM,8X,
     1                                          11HGAS TEMP, F
     1    ,8X,15HSORBENT TEMP, F      ,6X,15HCOOLANT TEMP, F    ,7X,15HHX CO
     2RE TEMP, F   )
  102 FORMAT(/(I9,2F12.4,5X,4(F14.4,6X)))
  202 FORMAT (//  38HLOADING AT INTERIOR OF SORBENT, LB/LB
     1                                         //4X,4HSORB/4X,4HNOD
     1E,3X, 3HAVG, 9X,
     1      1H1,9X,1H2,9X,1H3,9X,1H4,9X,1H5,9X,1H6,9X,1H7,9X,
     21H8,9X,1H9,8X,2H10,
     28X,2H11/6H AXIAL/5H NODE)
  203 FORMAT ( I5,4X,12(F6.4,4X))
  204 FORMAT(/27HOTIME AVG CO2 ADSORP RATE =
     1    F8.4, 6H LB/HR ,10X,
     227H TIME AVG H2O ADSORP RATE =
     3  F8.4, 7H LB/HR               )
  205 FORMAT(/// 30H AVG CO2 LOADING IN M.S. BED = F8.4,1X,5HLB/LB,7X,
     130H AVG H2O LOADING IN S.G. BED = F8.4, 6H LB/LB)
  206 FORMAT( //21H TIME AVG EXIT PH2O =  , F10.4, 3H MM ,18X,
     140HTIME AVG RATE OF M.S. POISONING BY H2O = , G12.4,10H LB H2O/HR)
      END
```

@ ELT S9980,1,690501, 43789

```
      SUBROUTINE MDESOR
C     MAIN PROGRAM FOR TRANSIENT DESORPTION BED CALCULATIONS
C
      COMMON /BLOK1/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),E(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),WSG(41)
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
     1      CP1,CP2,X,DT
      DOUBLE PRECISION C1P,C2P,C3P,D1P
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      COMMON /BLOK10/ NPRINT,DTMAX,NDTCON
      COMMON /BLOK11/ TOTCO2,TOTH2O
      COMMON /BLOK13/ WI, TI
      COMMON /BLOK14/ NCYCLE
      COMMON /BLOK17/ NSTART
C
      TIME = 0.0
      DTO =0.0
      DT=1.E-5
      TOTCO2=0.0
      TOTH2O=0.0
      DO 20 N=1,NDX1
      TS1(N)= TS(N)
      TS2(N)= TS(N)
      TX2(N)=TX(N)
      TX1(N)=TX(N)
      TC1(N)=TC(N)
      TC2(N)=TC(N)
   20 CONTINUE
      CALL START
      CALL PRDESB
      NPR = 0
      GO TO 3
    2 CALL PRDESB
      IF( TIME .GE. CYCLE) GO TO 9999
      NPR = 0
    4 CONTINUE
      DTO=DT
      GO TO (41,42),NDTCON
   41 ADT=DTMAX
      DO 60 N=1,NDX1
      ADT2=WI     /(ABS(W(NDR4,N)+WS(N))+1.E-9)*DT
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TS(N)-TS2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TX(N)-TX2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TC(N)-TC2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
```

```
   60 CONTINUE
      DT=ADT
      GO TO 3
   42 DT=DTMAX/10.0
      IF(TIME .LT. 1.E-4) DT=DTMAX/1000.0
      IF(TIME .GT. 0.06) DT=DTMAX
    3 CONTINUE
      IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
      DO 21 N=1,NDX1
      TS2(N)=TS1(N)
      TS1(N)=TS(N)
      TX2(N)=TX1(N)
      TX1(N)=TX(N)
      TC2(N)=TC1(N)
      TC1(N)=TC(N)
   21 CONTINUE
      D9=DT
      CALL DESORB(D9)
      TOTCO2=TOTCO2+DT*FR(1,NDX1)*WM(1)
      TOTH2O=TOTH2O+DT*FR(2,NDX1)*WM(2)
      TIME=TIME+DT
      NPR=NPR+1
      IF( (NPR.GE. NPRINT) .AND. (NCYCLE .GE. NSTART) ) GO TO 2
      IF(TIME .GE. CYCLE) GO TO 2
      GO TO 4
 9999 CONTINUE
      RETURN
      END
```

```
@ ELT S9981,1,690501, 43789

        FUNCTION IFN(N,NDXM)
        IFN=1
        IF(N.GT.NDXM)IFN=2
        RETURN
        END
```

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@ ELT S9983,1,691016, 39084    , 1
      SUBROUTINE DESORB(DELT)
C
      COMMON /BLOK1/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,G,DPKDTS,
     1DPKDWK,CP1,CP2,X,DT
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK4/ POUT(10),TIMET(10),NBCOUT,NPSET(3)
      COMMON /BLOK12/ NTEMP
      DIMENSION AS(2),PD(41)
      DIMENSION P4(41),VIST(2)
      DOUBLE PRECISION PD
      DOUBLE PRECISION C1P,C2P,C3P,D1P
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS)
      DATA VIST/0.014,0.009/
      DT=DELT
      AS(1)=4.*3.1416*RS(1)**2
      AS(2)=4.*3.1416*RS(2)**2
C
C
C
      DATA RGAS/554./
C
      NDR=NDR4-1
      DO 21 N=1,NDX1
      J=2
      P4(N)=PT(N)
      I=IFN(N,NDXM)
      IF( I .EQ. 2) J=1
      VIS= X(N)*VIST(I)+(1.-X(N))*VIST(J)
      F(N)=2.494E-4*PT(N)**0.795*(VIS/0.0174)
      DO 20 NR=1,NDR4
      C1(NR,N)=-CR2(I,NR)
      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
   20 C3(NR,N)=-CR3(I,NR)
C
C
      B(1,N)=C3(1,N)/C2(1,N)
      DO 21 J=2,NDR
   21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
      NDX=NDX1-1
C     TO TEMPORARILY STORE SURFACE LOADING
      DO 50 N=1,NDX1
   50 WS(N)=W(NDR4,N)
C
C     TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
      IF(NTEMP.EQ.0) GO TO 111
```

```
      DO 12 N=1,NDX1
      I=IFN(N,NDXM)
      CS2(N)=DT/CPS(N)/RHOSB(N)*ASG(N)*GK(N)*WM(I)*DH(N)
      CS1(N) = CS2(N)*X(N)
      IF(N.EQ.1) S1=((ABED(N)+ABED(N+1))*SK(N+1)*(TS(N+1)-TS(N)))/(2.*
     1     ABED(N)*DX*DX)
      IF(N.EQ.1) GO TO 15
      S1=((ABED(N-1)+ABED(N))*SK(N)*(TS(N-1)-TS(N))+(ABED(N)+ABED(N+1))
     1     *SK(N+1)*(TS(N+1)-TS(N)))/(2.*ABED(N)*DX*DX)
   15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+
     1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
      RATIO = (DT+DTO)/DT
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=RATIO*CS1(N)/(1.+T1)
      CS2(N)=RATIO*CS2(N)/(1.+T1)
      DS(N)=RATIO*DS(N)
      DS(N)= (DS(N)+T1*TS2(N))/(1.+T1)
   12 CONTINUE
      GO TO 110
  111 DO 112 N=1,NDX1
      CS1(N)=0.
      CS2(N)=0.
      DS(N)=0.
      TS(N)=T268
      TC(N)=T268
      TX(N)=T268
      TG(N)=T268
  112 CONTINUE
  110 CONTINUE
C
C     TO CALCULATE TOTAL PRESSURE
C
      DO 24 N=1,NDX1
      I=IFN(N,NDXM)
C     TO CALCULATE P1,P2,P3
      WSURF=W(NDR4,N)
      PSURF=PKEQ(I,WSURF,TS2(N))                                        *NEW
      DPKDTS=                                                           **-1
     1      (PKEQ(I,WSURF    ,(TS2(N)+0.001))-PSURF             )/      *NEW
     20.001                                                             **-1
      DPKDWK=(PKEQ(I,(WSURF    +1.E-6),TS2(N))-PSURF              )/1   *NEW
     1.E-6                                                              **-1
      G=1.+CS2(N)*DPKDTS
      P1(N)=(PSURF                    +DS(N)*DPKDTS)/G
      P2(N)=DPKDWK/G
      P3(N)=CS1(N)/G*DPKDTS
C
      C2(NDR4,N)=CR1(I,NDR4)/DT+CR2(I,NDR4)+WM(I)*GK(N)*P2(N)*AS(I)
      C3(NDR4,N)=0.0
      DO 23 NR=1,NDR4
   23 D1(NR,N)=CR1(I,NR)/DT*W(NR,N)
      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(I)
      D2(N)=AS(I)*WM(I)*GK(N)*(X(N)    -P3(N))
      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))
      Q(1,N)=D1(1,N)/C2(1,N)
      DO 24 J=2,NDR4
   24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
C
C     COEFFICIENTS FOR P-EQUATION
```

```
      DO 25 N=2,NDX
   25 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1
     1)/F(N+1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(2.*DX)
      N=1
      PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1
     1)/F(N+1) - VOIDF(N  )*C(N  )*ABED(N  )/F(N  ))/(1.*DX)
      N= NDX1
      PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N  )*C(N  )*ABED(N
     1)/F(N  ) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(1.*DX)
      DO 26 N=1,NDX1
      PC1(N)=PT(N)/F(N)
   26 PC3(N)=PT(N)/C(N)/VOIDF(N)*ASG(N)*GK(N)
C
      DO 27 N=1,NDX1
      CP1(N)=PC3(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
      CP2(N)=PC3(N)*(P2(N)*D2(N)+P3(N)      -X(N))
      C1P(N)=-PC1(N)/DX/DX+PC2(N)/2./DX
      C2P(N)=1./DT+2.*PC1(N)/DX/DX-CP2(N)
      C3P(N)=-PC1(N)/DX/DX-PC2(N)/2./DX
   27 D1P(N)=PT(N)/DT+CP1(N)
C
C     BOUNDARY CONDITION FOR P-EQUATION
C
      C2P(1)=C2P(1)+C1P(1)
      C1P(1)=0.
      GO TO (55,56), NBCOUT
   55 CONTINUE
      PTNDX1=PT(NDX1)/0.888
      CEXIT=(ALOG(PTNDX1)+1.76)/(1.96*PT(NDX1))/(VOIDF(NDX1)*RHOG(NDX1)
     1      *ABED(NDX1))
      C2P(NDX1) = C2P(NDX1)+C3P(NDX1)*(1.-DX*F(NDX1)*CEXIT)
      C3P(NDX1)=0.0
      GO TO 57
   56 CONTINUE
C  PRESSURES ARE SET
C
      DO 561 K= 1, 3
      IF(NPSET(K) .EQ. 0) GO TO 561
      NP=NPSET(K)
      C1P(NP)=0.0
      C2P(NP)=1.0
      C3P(NP)=0.0
      CALL LAGIN2(10,TIMET,10,2,TIME,D1PNP   ,POUT)
      D1P(NP)=D1PNP
  561 CONTINUE
   57 CONTINUE
      CALL FDEGID(C1P,C2P,C3P,D1P,PD,NDX1)
      DO 34 N=1,NDX1
      IF(PD(N) .LE. 0.) PD(N) = 1.E-3
   34 PT(N)=PD(N)
C
C     TO CALCULATE SORBENT LOADING
C
      DO 30 N=1,NDX1
      W(NDR4,N)=Q(NDR4,N)+D2(N)*PT(N)
      DO 30 J=2,NDR4
      L=NDR4+1-J
   30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
C
C     TO CALCULATE STREAM COMPOSITION
```

```
C
      FR(1,1) = 0.0
      FR(2,1)=0.
      FR2=0.0
      DO 31 N=1,NDX1
      I=IFN(N,NDXM)
      TEMP    =C(N)*VOIDF(N)
     1/P4(N)*ABED(N)                   *DX*(CP1(N)+CP2(N)*PT(N))
      IF(I.EQ.1)J=2
      IF(I.EQ.2)J=1
      IF(N . EQ. 1) GO TO 200
      FR(J,N)=FR(J,N-1)
      FR(I,N)=TEMP+FR(I,N-1)
      IF( NDXM .EQ. 0) GO TO 202
      IF (I .EQ. 1) GO TO 202
      IF(NPSET(2) .NE. 0) GO TO 202
      GO TO 201
  200 FR(I,1) = TEMP
  202 X(N) = 1.0
      GO TO 31
  201 CONTINUE
      CT=ABED(N)*DX*ASG(N)*GK(N)
      FRT= FR(1,N)+FR(2,N)+1.E-10
      PSURF = P1(N)+P2(N)*(W(NDR4,N)-WS(N))+P3(N)*PT(N)
      X(N)=((FR(2,N-1)+CT*PSURF                                  )/FRT/
     1 (1.+CT*PT(N)/FRT)      )
      IF(X(N) .LT. 0.0) X(N)=0.0
      IF(X(N) .GT. 1.0) X(N)=1.0
   31 CONTINUE
      DO 33 N=1,NDX1
      C(N) = (PT(N)/RGAS/(TG(N)+460)+C(N))/2.0
      I = IFN (N,NDXM)
      IF (I.EQ.1) J=2
      IF (I.EQ.2) J=1
      RHOG(N)=C(N)*(X(N)*WM(I)+(1.-X(N))*WM(J))
      UG(N)=(FR
     1        (1,N)*WM(1)+FR(2,N)*WM(2))/RHOG(N)/ABED(N)/VOIDF(N)
   33 CONTINUE
      IF( NTEMP .EQ. 0) RETURN
C
C     TO CALCULATE SORBENT TEMPERATURES
      CALL TSCRB
C
      D9=DT
      CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,D9,AVC,NOG)
      CALL HXCORE(TX,TC,TS,TG,HXC,HXS,HXG,RHOX,CPX,TKX,DX,D9,NDX1,AVX,
     1NDXM)
      CALL GAST(DX,RHOG,CPG,UG,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF)
  100 FORMAT(8G12.3)
      RETURN
      END
```

```
@ ELT S9984,1.690501, 43794

      SUBROUTINE FDEQIM(C1,C2,C3,D,VAR,NN)
      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
      NN1=NN-1
      B(1)=C3(1)/C2(1)
      DO 41 J=2,NN1
   41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
      Q(1)=D(1)/C2(1)
      DO 42 J=2,NN
   42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
      VAR(NN)=Q(NN)
      DO 43 J=2,NN
      L=NN+1-J
   43 VAR(L)=Q(L)-B(L)*VAR(L+1)
      RETURN
      END
```

```
@ELT S9985,1,690581, 43795
      SUBROUTINE FDEQID(C1,C2,C3,D,VAR,NN)
      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
      DOUBLE PRECISION C1,C2,C3,D,VAR,B,Q
      NN1=NN-1
      B(1)=C3(1)/C2(1)
      DO 41 J=2,NN1
   41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
      Q(1)=D(1)/C2(1)
      DO 42 J=2,NN
   42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
      VAR(NN)=Q(NN)
      DO 43 J=2,NN
      L=NN+1-J
   43 VAR(L)=Q(L)-B(L)*VAR(L+1)
      RETURN
       END
```

• ELT S9986,1,690501, 43796

```
      SUBROUTINE GAST (DX,RHOG,CPG,U,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF
     1)
      DIMENSION RHOG(1),CPG(1),U(1),TS(1),TX(1),TG(1),ASG(1),HSG(1),HXG(
     11),VOIDF(1),AXG(1)
      W=1.0
      N2= NDX1-1
      TG(1)=TS(1)
      DO 10 N= 1, N2
      F= 0.5*(VOIDF(N)+ VOIDF(N+1))
      AS1=ASG(N+1)
      HS1=HSG(N+1)
      AX1=AXG(N+1)
      HX1=HXG(N+1)
      CP1=CPG(N)
      RO = 0.5*(RHOG(N)+RHOG(N+1))
      U1= 0.5*( U(N)+U(N+1))
      TS1=TS(N+1)
      TX1=TX(N+1)
      C1=1./(F*RO*CP1*U1)
      D=C1*(AS1*HS1*TS1+AX1*HX1*TX1)
      A=(AS1*HS1+AX1*HX1)*C1
   10 TG(N+1)=((1./DX-A*(1.-W))*TG(N)+D)/(1./DX+A*W)
      RETURN
      END
```

```
@ ELT S9987,1,690501, 43797
      SUBROUTINE TGLCOL(TC,NDXMAX,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
     1AVC, NOGLIN)
      DIMENSION C1(41),C2(41),C3(41),D(41),TC(1),TX(1),HXC(1),AVC(1),B(4
     11),Q(41)
      DIMENSION UC(1),RHOC(1),CPC(1),AXC(1)
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      DN=DT*DTO
      DO 10 N= NOGLIN,NDXMAX
      CC1=-UC(N)
      CC2=HXC(N)/(CPC(N)*RHOC(N))*AVC(N)*0.5
      IF( UC(N) .GT. 0.) GO TO 5
      C3(N)=-CC1/DX
      C2(N)=1./DN+CC2-C3(N)
      C1(N)=0.0
      GO TO 10
    5 C1(N) = CC1/DX
      C2(N) = 1./DN + CC2 - C1(N)
      C3(N) = 0.0
   10 D(N)=TC2(N)/DN+CC2*TX1(N)*2. - CC2*TC2(N)
      C1(NOGLIN) = 0.
      C3(NOGLIN) = 0.
      D(NOGLIN)=D(NOGLIN) +ABS(UC(NOGLIN))/DX*T268
      NOG2=NOGLIN-1
      DO 51 N= 1, NOG2
   51 TC(N)=0.00
      NN=NDXMAX
      NN1=NN-1
      N1=NOGLIN
      N2=N1+1
      B(N1)=C3(N1)/C2(N1)
      DO 41 J=N2,NN1
   41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
      Q(N1)=D(N1)/C2(N1)
      DO 42 J=N2,NDXMAX
   42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
      TC(NN)=Q(NN)
      DO 43 J= N2,NN
      L=NN+N1-J
   43 TC(L)=Q(L)-B(L)*TC(L+1)
      RETURN
      END
```

@ ELT S998B,1,690617, 53903 T1

```
      SUBROUTINE START
C
      COMMON /BLOK1/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
     1    CP1,CP2,X,DT
      DOUBLE PRECISION C1P,C2P,C3P,D1P
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
C
      IST=NDX1-NDXM
      DMF=0,8/IST
      RS(1)=RHOSB(1)*3./RHOS(1)/ASG(1)
      RS(2)=RHOSB(NDX1)
     1              *3./RHOS(2)/ASG(NDX1)
      DO 30 N= 1, NDX1
      RHOG(N) = 0.0003
      X(N)=1.0
      ID=IFN(N,NDXM)
      IS=N-NDXM
      IF(ID.EQ.2) X(N)=IS*DMF
      C(N) = 0,2E-3
      PT(N)=6.00
      I= IFN(N,NDXM)
   30 VOIDF(N) = 1. - RHOSB(N)/RHOS(I)
      X(NDXM+1)=0.01
      NDR=NDR4-1
      NDR2=2.*NDR
      NDR3=NDR2+1
      DO 10 I=1,2
      VS(I)=4./3.*3.1416*RS(I)**3
      DVS(I)=VS(I)/NDR
      DVS1(I)=DVS(I)/2
      RS1(I,1)=0.
      DO 10 K=2,NDR3
   10 RS1(I,K)=CBRT(3./4./3.1416*(4./3.*3.1416*RS1(I,K-1)**3+DVS1(I)))
      DO 11 I=1,2
      IF(I.EQ.1) DIF1=DIF(1)
      IF(I.EQ.2) DIF1=DIF(NDX1)
      CR1(I,1)=DVS1(I)*RHOS(I)
      CR2(I,1)=0.
      CR3(I,1)=4.*3.1416*RS1(I,2)**2*DIF1  /(RS1(I,3)-RS1(I,1))*RHOS(I)
      DO 11 K=2,NDR4
      CR1(I,K)=DVS(I)*RHOS(I)
      CR2(I,K)=4.*3.1416*RS1(I,2*K-2)**2*DIF1  /(RS1(I,2*K-1)-RS1(I,2*K-
     13))*RHOS(I)
   11 CR3(I,K)=4.*3.1416*RS1(I,2*K)**2*DIF1  /(RS1(I,2*K+1)-RS1(I,2*K-1)
     1)*RHOS(I)
      CR1(1,NDR4)=CR1(1,1)
      CR1(2,NDR4)=CR1(2,1)
```

```
      RETURN                                                       000059
      END                                                          000060
```

• ELI 69989,1,690501, 43800

```
      SUBROUTINE PROESB
C
C
      DIMENSION AVLD(41)
      COMMON /BLOK1/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,FR(2,41),RB(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDF(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      COMMON /BLOK3/ W(21,41),TB(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK4/ POUT(10),TIMET(10),NBCOUT,NPSET(3)
      COMMON /BLOK6/ NCYCLT
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      COMMON/BLOK10/ NPRINT,DTMAX,NDTCON
      COMMON /BLOK11/ TOTCO2,TOTH2O,SUMPTM,WTACMS,ITSG
      COMMON /BLOK12/ NTEMP
      COMMON /BLOK13/ WI, TI
      COMMON /BLOK14/ NCYCLE
      COMMON /BLOK16/ NDXMAC, RCOBC, VOLCAB, RCO2C
      COMMON /BLOK17/ NSTART
      DIMENSION AXS(41),AXG(41),AGS(41),HSX(41),HGX(41),HGS(41),ACX(41),
     1HCX(41)
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS),(AXC,ACX),(HXC,HCX)
      DOUBLE PRECISION C1P,C2P,C3P,D1P
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
     1     CP1,CP2,X,DT
      EQUIVALENCE(NDX,NDX1)
C
      TIMEM=60.*TIME
      WRITE (6,100) NCYCLE, TIME, TIMEM, DT
      WRITE (6,101)
      WRITE (6,102)(N,PT(N),TG(N),TS(N),TC(N),TX(N),N=1,NDX)
      IF(( NPSET(1) .GT. 0) .OR. (NPSET(2) .GT. 0)) GO TO 99
      WRITE (6,200)
      WRITE (6,201)(N,X(N),FR(1,N),FR(2,N),N=1,NDX)
   99 WRITE (6,202)
      N1=NDXM+1
      NDR3=NDR4-1
      DO 20 N= 1, NDXM
      SUMMS=0.0
      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
      IF(NDR4 .EQ. 2) AVLD(N) = SUMMS
      IF(NDR4.EQ.2) GO TO 20
      DO 22 NR=2,NDR3
   22 SUMMS=SUMMS+W(NR,N)
      AVLD(N)=SUMMS/NDR3
   20 CONTINUE
      DO 30 N= N1,NDX1
      SUMMS=0.0
      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
      IF(NDR4.EQ.2) AVLD(N) = SUMMS
```


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```
      IF(NDR4.EQ.2) GO TO 30
      DO 33 NR=2, NDR3
   33 SUMMS=SUMMS+W(NR,N)
      AVLD(N)=SUMMS/NDR3
   30 CONTINUE
      IF(NDXMAC .EQ. 0) GO TO 35
      SUM=0.
      DO 31 N= 1, NDXMAC
   31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVMSLD = SUM/WTACMS
   35 CONTINUE
      IF((NDX1-NDXM) .EQ. 0) GO TO 40
      SUM=0.
      DO 32 N= N1,NDX1
   32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVSGLD=SUM/WTSG
   40 CONTINUE
      DO 10 N=1,NDX
   10 WRITE (6,203)N, AVLD(N)
     1                ,(W(NR,N),NR=1,NDR4)
      WRITE (6,205) AVMSLD, AVSGLD
      IF(TIME .LT. 1.E-20) AVMSL1=AVMSLD
      IF(TIME .LT. 1.E-20) AVSGL1=AVSGLD
      AVRCO2=WTACMS*(AVMSL1-AVMSLD)/TIME
      AVRH2O=WTSG*(AVSGL1-AVSGLD)/TIME
      WRITE(6,204) AVRCO2,AVRH2O
      RETURN
C
  100 FORMAT (1H1,16HDESORPTION CYCLE  I3/
     1         3X,5HTIME=,F9.5,1X2HHR,F12.3,1X,3HMIN,
     1                                  5X,15HTIME INCREMENT=F7.5,1X2HHR)
  101 FORMAT (//2X,10HAXIAL NODE,10X,14HTOTAL PRESS,MM,6X,14HGAS TEMP,DE
     1G F,5X,19HSORBENT TEMP, DEG F,2X,18HCOOLANT TEMP,DEG F,3X,19HHX CO
     2RE TEMP, DEG F  )
  102 FORMAT(/(I9,11X,5(F14.4,6X)))
  103 FORMAT (/21HOCO2 DESORPTION RATE=F7.4,1X5HLB/HR,5X,20HH2O DESORPTI
     1ON RATE=F7.4,1X5HLB/HR)
  200 FORMAT (1HO/2X,10HAXIAL NODE,13X,9HMOLE FRAC,7X,
     12X,13HCO2 RATE,M/HR,6X,13HH2O RATE,M/HR)
  201 FORMAT(/(I9,11X,3(4X,F12.6,4X)))
  202 FORMAT (//  31HOLOADING AT INTERIOR OF SORBENT//4X,4HSORB/4X,4HNOD
     1E,3X, 3HAVG, 9X,
     1    1H1,9X,1H2,9X,1H3,9X,1H4,9X,1H5,9X,1H6,9X,1H7,9X,
     21H8,9X,1H9,8X,2H10,
     28X,2H11/6H AXIAL/5H NODE)
  203 FORMAT ( I5,4X,12(F6.4,4X))
  204 FORMAT(/27HOTIME AVG CO2 DESORP RATE =
     1    F8.4, 6H LB/HR ,10X,
     227H TIME AVG H2O DESORP RATE =
     3  F8.4, 7H LB/HR              )
  205 FORMAT(/// 30H AVG CO2 LOADING IN M.S. BED = F8.4,1X,5HLB/LB,7X,
     130H AVG H2O LOADING IN S.G. BED = F8.4, 6H LB/LB)
      END
```

322449

```
• ELT S9991.1.690501. 43801
      SUBROUTINE HXCORE(TX,TC,TS,TG,HXC,HXS,HXG,RHOX,CPX,TKX,DX,DT,NDX,A
     1VX,NDXM)
C
      DIMENSION TX(1),TC(1),TS(1),TG(1),HXC(1),HXS(1),HXG(1),RHOX(1),
     1CPX(1),TKX(1),AVX(1)
      DIMENSION C1(41),C2(41),C3(41),D1(41)
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      DN=DT+DTO
      DO 10 N=1,NDX
      T1= AVX(N)*(HXC(N)+HXS(N)+HXG(N))*0.5
      C1(N)=-TKX(N)/DX/DX
      C3(N)= -TKX(N+1)/DX/DX
      C2(N)= RHOX(N)*CPX(N)/DN -C1(N) - C3(N) + T1
   10 D1(N) = RHOX(N)*CPX(N)/DN*TX2(N) + AVX(N)*(HXC(N)
     1*TC1(N) + HXS(N)*TS1(N)+HXG(N)*TG(N)) - T1*TX2(N)
      C2(1)=C2(1)+C1(1)
      C1(1)=0.
      C2(NDX)=C2(NDX)+C3(NDX)
      C3(NDX)=0.0
      CALL FDEQIM(C1,C2,C3,D1,TX,NDX)
      RETURN
      END
```


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● ELT S9996,1,690501, 13802

```
      SUBROUTINE LAGIN2(ID,X,NP,ND,XO,YO,Y)
C     REVISED FOR FORTRAN IV 8-8-65  S. WONG
      DIMENSION  X(2),  Y(2)
C
      ILO=1
      IF(XO-X(1))10,16,4
    4 IF(XO-X(NP))19,13,7
    7 ILO=NP-1
   10 IHI=ILO+1
      WRITE (6,1) ID,XO
      GO TO 46
   13 ILO=NP
   16 YO=Y(ILO)
      RETURN
   19 DO 22 ILO=2,NP
      IF(XO-X(ILO))25,16,22
   22 CONTINUE
   25 IHI=ILO
      ILO=IHI-1
      IF(ND-2)46,46,28
   28 DO 43 I=3,ND
      IF(ILO-1)40,40,31
   31 IF(IHI-NP)34,37,37
   34 IF (2.*XO-X(ILO-1)-X(IHI+1)) 37,37,40
   37 ILO=ILO-1
      GO TO 43
   40 IHI=IHI+1
   43 CONTINUE
   46 YO=0.0
      PN=1.0
      DO 49 I=ILO,IHI
   49 PN=PN*(XO-X(I))
      DO 58 I=ILO,IHI
      P=PN/(XO-X(I))
      DO 55 J=ILO,IHI
      IF(J-I)52,55,52
   52 P=P/(X(I)-X(J))
   55 CONTINUE
      YO=YO+P*Y(I)
   58 CONTINUE
      RETURN
    1 FORMAT (97X,7HLAGIN2 ,I4,E12.5)
      END
```

```
@ ELT S9907,1,690501, 43804

      SUBROUTINE ISORB
      COMMON /BLOK1/ ABED(41), A(41), AVC(41),CPG(41),RHOG(41),
     1HXG(41),HXS(41),HXC(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
     2S1(2,41),RHOS(2),UG(41),WM(2),UC(41),NDXM,PS(41),RHOSB(41),DS(41),
     3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
     41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
     5,ER(2,41),BS(2),NDX1,NDR4,DX,DT,GK(41),DH(41),SK(41),P1(41),P2(41)
     6,P3(41),WS(41),CR1(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
     7Q(21,41),CP1(41),CP2(41),X(41),VOIDE(41),TIME
     8,AXC(41),RHOC(41),CPC(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
     9,NOG,PK(2,41),PCO2I,PH2OI,  GMR,GMW,TGI,PA,PT(41),CPS(41),HSG(41)
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
     1      CP1,CP2,X,DT
      DOUBLE PRECISION C1P,C2P,C3P,D1P
      COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
      DOUBLE PRECISION W
      COMMON /BLOK8/ DTO,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
      DIMENSION S1(41),S2(41),S3(41),B1(41)
      DO 10 N=1,NDX1
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=CS1(N)*(1.0+T1)
      CS2(N)=CS2(N)*(1.0+T1)
      B1(N) =TS2(N)+CS1(N)*PT(N)-CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)-WS(N))+
     1P3(N)*PT(N))+T*(ASG(N)*HSG(N)*TG (N)+ASX(N)*HXS(N)*
     2                                               TX1(N))-T1*TS2(N)
      IF(N.EQ.1) S1(N)=0.0
      IF(N.EQ.1) GO TO 11
      S1(N)=-T*SK(N)/DX/DX*(ABED(N-1)+ABED(N))/(2.*ABED(N))
   11 S3(N)=-T*SK(N+1)/DX/DX*(ABED(N)+ABED(N+1))/(2.*ABED(N))
      S2(N)=1.-S1(N)-S3(N)+T1
   10 CONTINUE
      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1)
      RETURN
      END

   END CUR       UCC 1/4
```

PART II

MULTIPLE BED PROGRAM (MAIN4B)

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NOMENCLATURE

FORTRAN	Algebraic*	Description
A	$\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g}\right)$	Quantity $\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g}\right)$ appearing in Equation (2-35), Ref (1) (lb-mole)/(hr)(sq ft)(mm Hg)
ADT		Temporary storage for DT, hr
ADT2		Temporary storage for DT, hr
ABED	A	Cross-sectional area of adsorbent bed, sq ft
AGS, ASG	a_{sg}	External surface area of sorbent, sq ft/(cu ft of bed)
AGX, AXG	a_{xg}	Primary heat transfer area between heat exchanger and gas stream, sq ft/cu ft of sorbent bed
ASX, AXS	a_{xs}	Primary heat transfer area between heat exchanger and sorbent, identical to a_{xg}
AVC	a_{vc}	Primary heat transfer area for coolant, sq ft/(cu ft of coolant volume)
AVLD		Average loading at each axial node, (lb-sorbate)/(lb-sorbent)
AVH2OP		Average poisoning rate of molecular sieves by H_2O, (lb-H_2O)/hr
AVMSLD		Average CO_2-loading of all active molecular sieve sorbents, lb-CO_2/(lb-molecular sieves)
AVPH2Ø		Average outlet P_{H_2O}, mm Hg
AVRCØ2		Average CO_2 adsorption or desorption rate, lb-CO_2/hr
AVRH2Ø		Average H_2O adsorption or desorption rate, lb-H_2O/hr
AVSGLD		Average H_2O-loading of desiccant sorbents, lb-H_2O/(lb-desiccant)
AVX	a_{vx}	Primary heat transfer area for heat exchanger, sq ft plate area/(cu ft of metal)

*Referring to equations in Part I of this report.

FORTRAN	Algebraic	Description
B		Temporary variable used in simultaneous solution of a system of finite difference equations. See Equations (2-41) and (2-42), in Part I of this report.
C	C	Molal density of gas mixture, lb moles/(cu ft)
CPC	C_{pc}	Heat capacity of coolant, Btu/(^{o}F)(lb)
CPG	C_{pg}	Heat capacity of gas mixture, Btu/(^{o}F)(lb)
CPL		Specific heat of adsorbed sorbate, Btu/(^{o}F)(lb)
CPP		Specific heat of dry sorbent, Btu/(^{o}F)(lb)
CPS	C_{ps}	Sorbent specific heat, Btu/(lb)(^{o}F)
CPX	C_{px}	Heat capacity of heat exchanger metal, Btu/^{o}F)(lb)
CP1 CP2		Coefficients in equation $PC3 \cdot \left(P_{ks_{t+\Delta t}}\right) - X_k P_{t+\Delta t} = CP1 + CP2 \cdot P_{t+\Delta t}$
CR1 CR2 CR3		Coefficients in following equation which is merely another form of Equation (2-28), in Part I of this report. $CR1 \cdot \frac{W_{k,M,(t+\Delta t)} - W_{k,M,t}}{(\Delta t)} = CR2 \cdot \left(W_{k,(M-1)(t+\Delta t)} - W_{k,M,(t+\Delta t)}\right) + CR3 \cdot \left(W_{k,M,(t+\Delta t)} - W_{k,(M+1),(t+\Delta t)}\right)$
CS1 CS2		Coefficients in equation $T_{s(t+\Delta t)} - T_{s,t} = DS + CS1 \cdot P_{(t+\Delta t)} - CS2 \cdot P_{ks,(t+\Delta t)}$
CYCLE		Cycle time per one adsorption or one desorption half-cycle, hr
C1 C2 C3		Coefficients in equation $C_1 \cdot W_{(t+\Delta t),(M-1)} + C2 \cdot W_{(t+\Delta T),M} + C3 \cdot W_{(t+\Delta t),(M+1)} = D1$

FORTRAN	Algebraic	Description
C1P		Coefficients in equation $C1P \cdot P_{(t + \Delta t), (N-1)} + C2P \cdot P_{(t + \Delta t), N} + C3P \cdot P_{(t + \Delta t), (N + 1)} = D1P$
C2P		(see C1P)
C3P		(see C1P)
DH	ΔH	Heat of adsorption at each node Btu/(lb adsorbed)
DIF	D_k	Mass diffusivity of component k through the interior of sorbent, sq ft/hr
DP		Sorbent diameter, ft
DPCØ2C		Cabin CO_2 partial pressure increase in one time increment, mm Hg
DS		See CS1
DT	Δt	Time increment, hr
DTMAX		Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
DTØ		Time increment of previous computation step, hr
DTT		Maximum allowable time increment calculated from each bed transient, hr
DVS		Size of interior sorbent volume elements, (cu ft)
DVS1		Size of sorbent volume elements at surface and center of spherical pellets, DVS1 = 1/2 DVS, (cu ft)
DX		Axial node dimension, ft
D1		See C1
D1P		See C1P
D2		Coefficient in equation $W_{ks(t + \Delta t)} = Q + D2 \cdot P_{(t + \Delta t)}$
F	F	Factor defined by Equation (2-17), a function of pressure
FR		Molal flow rates of CO_2 and H_2O, during desorption, *FR (1,N) is CO_2 rate, FR (2,N) is H_2O rate, lb-mole/hr*

FORTRAN	Algebraic	Description
	G	Mass flux = $u_g \cdot \rho_g$, lb/(hr)(sq ft void area)
GK	K_g	Mass transfer coefficient between bulk stream and the surface of adsorbent. Surface kinetic rate can be incorporated in this coefficient, lb-moles/(hr)(sq ft)(mm Hg)
GMR	G_t	Total mass flow rate, lb/(hr)
GMR1 GMR2 GMR3 GMR4		GMR for bed 1, bed 2, bed 3 and bed 4, respectively
GMW	M_g	Average molecular weight of process gas
GMW1 GMW2 GMW3 GMW4		GMW for bed 1, bed 2, bed 3, and bed 4, respectively
HCX, HXC	h_{xc}	Heat transfer coefficient between heat exchanger primary plate and coolant, Btu/(sq ft)(^{0}F)(hr)
HGS, HSG	h_{sg}	Heat transfer coefficient between sorbent and gas, based on a_{sg}, Btu/(sq ft)(^{0}F)(hr)
HXS, HXS	h_{xs}	Effective heat transfer coefficient between heat exchanger primary plate and sorbent, Btu/(sq ft)(^{0}F)(hr)
HTR		Same as HTR1 if ISTØPC = 0. This variable is used in program
HTR1		Electric heater power read-in for each node, Btu/hr
HXG		Heat transfer coefficient between heat exchanger primary plate and gas stream, Btu/(sq ft)(^{0}F)(hr)
IDB		Storage variable for all the integer variables characterizing desiccant bed configurations, such as NPSET, NDR4, etc
IDSØRB		Index identifying sorbent used for each node; 1 = 5A, 2 = S.G. 3 = 13 X, 4 = 4A, 5 = 3A
IMAIN		Storage variable for the control integer variables for the system, such as NCYCLT, NPRINT, etc

FORTRAN	Algebraic	Description
IMB		Storage variable for all the integer variables characterizing molecular sieve bed configurations, such as NPSET, NDR4, etc.
ISTØPC		Control index showing availability of coolant and heat, if ISTØPC ≠ 0, WC = 0, HTR = 0, SABCØ2 = 0
KBED		Integer indicating whether a bed exists. KBED (3) = 0 means bed 3 does not exist
NCT1		Number of cycles to be run before assessment of water poisoning effects
NCT2		Number of cycles to be run after node adjustment for effects of water-poisoning
	$\dot{M}_{sg}$	Molal rate of mass transfer into bulk gas stream/unit bed volume, lb-moles per (cu ft of bed) (hr); see Equation (2-15), in Part I of this report.
	M_s	Interior node corresponding to the surface of pellet
NBCØUT		Integer control variable, if NBØUT = 2, the outlet manifold pressure is specified as a function of time; NBØUT = 1, the manifold pressure is computed from vacuum duct resistance
NCYCLE		Number of complete adsorption-desorption cycles from beginning of run
NCYCLT		Total number of complete adsorption-desorption cycle calculations desired
NDR4		Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDTCØN		If = 1, internal Δt calculations. If = 2, fixed Δt's in program will be used
NDXM		Integer denoting total number of molecular sieve nodes
NDXMAC		Integer denoting number of active molecular sieve modes, i.e., (NDXM-NDXMAX) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NDX1		Integer denoting total number of axial nodes

FORTRAN	Algebraic	Description
NHALF		NHALF = 1, beds 1 and 2 are adsorbing, beds 3 and 4 are desorbing; NHALF = 2, beds 1 and 2 are desorbing, and beds 3 and 4 are adsorbing
NØG		Node to which coolant is added
NPR		Number of time steps elapsed since last printout
NPRINT		Integer control variable which determines the frequency of printout occurrence; e.g., if NPRINT = 5, printout occurs after every five time steps
NPSET		Integers which denote the nodes to which tabulated vacuum history is applicable
NSTART		Integer denoting the cycle from which on bed performance will be printed at frequency specified by NPRINT
NST1		NSTART for the NCT1 run
NST2		NSTART for the NCT2 run
NTEMP		Integer control variable; if NTEMP = 0, the energy equations will be ignored and bed temperatures set equal to TCIN; if NTEMP ≠ 0, heat balances will be performed
PA	P	Bed total pressure during adsorption, mm Hg
PAC		Cabin pressure, mm Hg
PA1 PA2 PA3 PA4		PA for bed 1, bed 3, bed 3 and bed 4, respectively
PCØ2A		CO_2-accumulator pressure, psia
PCØ2C		CO_2 partial pressure in cabin, mm Hg
PCØ2I		CO_2 partial pressure at adsorption bed inlet, mm Hg
PCØ2I1 PCØ2I2 PCØ2I3 PCØ2I4		PCØ2I for bed 1, bed 2, bed 3 and bed 4, respectively

FORTRAN	Algebraic	Description
PC1 PC2 PC3		Coefficients in equation for desorption pressure $\frac{P_{(t+\Delta t), N} - P_{t, N}}{(\Delta t)}$ $= PC1 \cdot \frac{P_{(t+\Delta t), N-1)} - 2P_{(t+\Delta t), N} + P_{(t+\Delta t), (N-1)}}{(\Delta x)^2}$ $+ PC2 \cdot \frac{P_{(t+\Delta t), (N+1)} - P_{(t+\Delta t), (N-1)}}{2(\Delta x)}$ $+ PC3 \cdot \left[P_{ks(t+\Delta t)} - X_k P_{(t+\Delta t)}\right]$
PH2ØC		H_2O partial pressure in the cabin, mm Hg
PH2ØI		Inlet H_2O partial pressure, mm Hg
PH2ØI1 PH2ØI2 PH2ØI3 PH2ØI4		PH2ØI for bed 1, 2, 3 and 4, respectively
PK(K,N)	p_k	$p \cdot X_k$; partial pressure of component k in bulk gas stream, mm Hg
PK1 PK2 PK3 PK4		PK for bed 1, 2, 3 and 4, respectively
PN2		N_2 partial pressure for overboard loss computation
PN21 PN22 PN23 PN24		PN2 for bed 1, 2, 3 and 4, respectively
PØUT		10 tabulated desorption outlet pressures at TIMET, mm Hg
PØ2		O_2 partial pressure for overboard loss calculations
PØ21 PØ22 PØ23 PØ24		$PØ_2$ for bed 1, 2, 3, and 4, respectively
PS		Variable for a temporary storage of PT

FORTRAN	Algebaric	Description
PT	P	Total pressure in bulk gas stream, mm Hg
PT1 PT2 PT3 PT4		PT for bed 1, 2, 3 and 4, respectively
PUMP		Pressure ratios at which vacuum pump displacements VPUMP are tabulated
P1 P2 P3		Coefficients in equation $p_{ks_{(t+\Delta t)}} = P1 + P2 \cdot \left(W_{k,s(t+\Delta t)} - W_{k,s,t}\right) + P3 \cdot P$
Q		Temporary variable like B. See Equations (2-43) and (2-44), Ref (1)
RB1M		Variable equivalent to TG1, PH2ØI1, etc
RB2M		Variable equivalent to TG2, PH2ØI2, etc
RB3M		Variable equivalent to TG3, PH2ØI3, etc
RB4M		Variable equivalent to TG4, PH2ØI4, etc
RCØ2C		Rate of CO_2 generation in cabin, lb CO_2 per hr
RDB		Storage variable for real variables characterizing desiccant bed configuration
RDBA		Storage variable for real variables characterizing desiccant bed adsorption half cycle transfer processes
RDBD		Similar to RDBA for desorption half-cycles
RGAS	R	Gas constant, 554 (mm Hg) (cu ft)/(lb-mole)(^{o}R)
RHØC	ρ_c	Coolant density, lb/(cu ft)
RHØG	ρ_g	Gas density, lb/(cu ft)
RHØS	ρ_s	Sorbent density, lb/(cu ft particle)
RHØSB	ρ_{sb}	Sorbent bulk density, lb/(cu ft bed volume)
RHØX	ρ_x	HX core metal density, lb/(cu ft)

FORTRAN	Algebraic	Description
RMAIN		Real variable equivalent to WM, CYCLE, etc., which are common to all beds
RMB		Storage variable for real variables characterizing molecular sieve bed configuration, such as ABED, AVC, etc.
RMBA		Storage variable for real variables characterizing molecular sieve bed transfer processes during adsorption half cycles, such as HXG, HXS, etc.
RMBD		Similar to RMBA for desorption half cycles
RS	r_s	Average particle radius found from ρ_{sb} and a_{sg}, ft
RSI		Radius of spherical surface separating two interior sorbent volume elements, ft
SABCØS		A permanent storage for SABCØ2
SABCØ2		Rate of CO_2 intake by a Sabatier reactor or equivalent, lb/hr
SK	k_s	Effective thermal conductivity of sorbent bed, Btu/(hr) (sq ft) (°F/ft)
SUMPTM		Quantity $\sum_{t = zero}^{t} P_{H_2O,\ outlet} \cdot (\Delta t)$, (mm)(hr)
TC	T_c	Coolant temperature, °F
TCØ2A		CO_2-accumulator temperature, °F
TCIN		Identical with T268, inlet coolant temperature, °F
TCO1 TCO2 TCO3 TCO4		Initial TC for bed 1, 2, 3 and 4, respectively
TCI		Coolant temperature at time, t - Δt
TCI1 TCI2 TCI3 TCI4		TCI for bed 1, 2, 3, and 4, respectively

FORTRAN	Algebraic	Description
TC2		Coolant temperature at time, t - 2Δt
TC21 TC22 TC23 TC24		TC2 for bed 1, 2, 3 and 4, respectively
TG	T_g	Gas temperature, ^0F
TGC		Cabin temperature, ^0F
TGHX		Maximum allowable temperature at molecular sieve bed inlet, above which an intercooler will be used to lower it to TGHX, ^0F
TGI	T_{gi}	Inlet gas temperature for adsorption cycle, ^0F
TGI1 TGI2 TGI3 TGI4		TGI for bed 1, 2, 3, and 4, respectively
TG1 TG2 TG3 TG4		TG for bed 1, 2, 3, and 4, respectively
TI		Maximum temperature change allowable per time increment in selecting Δt, ^0F
TIME	t	Time from beginning of each adorption or desorption period, hr
TIMEDS		Maximum desorption time beyond which ISTØPC will be set equal to 1, hr.
TIMEM		Time above in minutes
TIMET		10 times at which PØUT are tabulated, hr
TKX	k_x	Thermal conductivity of heat exchanger core metal, Btu/(hr) (sq ft) (^0F/ft)
TMAX		Maximum allowable sorbent temperature, above which heater will be shut off, ^0F
TØTCØ2		Total amount of CO_2 adsorbed since beginning of adsorption period, lb

FORTRAN	Algebraic	Description
TØTHTC		Total heat added/removed by coolant, Btu
TØTH2Ø		Total amount of H_2O adsorbed since beginning of adsorption period, lb
TØTKWH		Total KWH of electric power used by desorbing beds, KWH
TS	T_s	Sorbent temperature, ^0F
TS01 TS02 TS03 TS04		Initial sorbent temperatures for bed 1, 2, 3, and 4, respectively
TS1		Sorbent temperature at time t - (Δt), ^0F
TS11 TS12 TS13 TS14		TS1 for bed 1, 2, 3, and 4, respectively
TS2		Sorbent temperature at time t-2 (Δt), ^0F
TS21 TS22 TS23 TS24		TS2 for bed 1, 2, 3, and 4, respectively
TX	T_x	Heat exchanger core metal temperature, ^0F
TX01 TX02 TX03 TX04		Initial TX for bed 1, 2, 3, and 4, respectively
TX1		Heat exchanger core metal temperature at time t - (Δt), ^0F
TX11 TX12 TX13 TX14		TX1 for bed 1, 2, 3, and 4, respectively
TX2		Heat exchanger core metal temperature at time t-2 (Δt), ^0F
TX21 TX22 TX23 TX24		TX2 for bed 1, 2, 3, and 4, respectively

FORTRAN	Algebraic	Description
T268	T_{268}	Inlet coolant temperature, ^0F
UC	u_c	Coolant velocity, ft/hr
UG	u_g	Interstitial gas velocity, i.e., true gas velocity, ft/hr
VCØ2A		CO_2-accumulator volume, cu ft
VMS		Total bulk volume of molecular sieve sorbents, cu ft
VØIDF	f	Void fraction of bed
VØLCAB		Cabin volume for atmosphere, cu ft; use VØLCAB = 10^{20}, for constant PCØ2C
VPUMP		Vacuum pump displacements tabulated at pressure ratios PUMP, cfm
VS		Volume of a single sorbent pellet, cu ft
VSG		Total bulk volume of desiccants, cu ft
W	W_k	Local loading of component k in sorbent, lb sorbate k/lb sorbent
WC		Coolant flow rate actually used in program, lb/hr
WCC		Coolant flow rate inputted, lb/hr
	$W_d(P)$	A function of pressure which represents the capacity of vacuum duct at duct inlet pressure of P mm, lb/hr
WI		Maximum loading change allowable per time increment in selecting Δt, lb/lb
WM	M_k	Molecular weight of component K. K = 1 and 2
WS		Temporary storage variable for W
WTACMS		Total weight of active molecular seive sorbents, lb
WTMS		Total weight of molecular sieve sorbents, lb
WTSG		Total weight of desiccants, lb
W1 W2 W3 W4		W for bed 1, 2, 3 and 4, respectively

FORTRAN	Algebraic	Description
X	x_k	Mole fraction of component k in gas stream k = 1 refers to CO_2 in molecular sieve bed gas stream, and K = 2 refers to H_2O in desiccant bed gas stream
	x	Distance from moelcular sieve bed end, ft
	Y	Any of bed properties, T_s, T_x, W_k, T_c, T_g

Subscripts

b	Bulk
c	Coolant
g	Gas stream
i	Inlet
k	Component k
M	Radial location index for sorbent interior nodes
N	Axial location index
s	Surface of sorbent
s	Sorbent
t	At time t
v	Volume
x	Heat exchanger

Superscripts

*	Equilibrium quantity

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SECTION 6

GENERAL DESCRIPTION

INTRODUCTION

The AiResearch composite sorbent bed program S9960 (Part I of this report) was developed for analyzing vacuum-dump sorbent bed systems such as the RCRS (Regenerative Carbon Dioxide Removal System) for the Apollo Applications Program and the Airlock Program. More complicated systems are required for longer mission applications in which H_2O, CO_2, or both must be saved. To accommodate more complex systems, program S9960 has been modified and expanded. The new program is identified as MAIN4B and will now accommodate 4-bed/H_2O-save-CO_2-dump and 4-bed/H_2O-save-CO_2-dump configurations as well as the original 2-bed/vacuum-dump configuration. A typical 4-bed thermal-swing system that uses coolant is shown in Figure 6-1.

Computational schemes of program MAIN4B are basically the same as those of program S9960, although modifications have been made and a number of new features added. These changes are described in Section 7, Technical Description.

The most significant new feature of program MAIN4B is prediction of the effects of coadsorption of water, CO_2, oxygen, and nitrogen on the system beds. The gradual buildup of water on the CO_2 removal bed has a pronounced effect of lowering the adsorption efficiency of that bed. Methods have been incorporated into MAIN4B to quantitatively predict this coadsorption effect. Also important is that coadsorption of atmospheric gases, oxygen and nitrogen, leads to loss of the gases overboard from a vehicle when vacuum-dump systems are employed. The rate of loss of these gases is estimated as a function of process conditions.

PROGRAM INPUT

The input to MAIN4B is by means of eleven namelists. The lists include initial conditions, bed sizes, mass and heat transfer coefficients, etc. However, equilibrium data of various sorbate-sorbent pairs are all contained in subroutines EQPWT and FCØAD in the form of data statements. These may have to be changed if better data become available.

PROGRAM OUTPUT

Printed pages are the only output from the program. The output provides the following:

(a) Bed size

(b) Estimated overboard gas losses

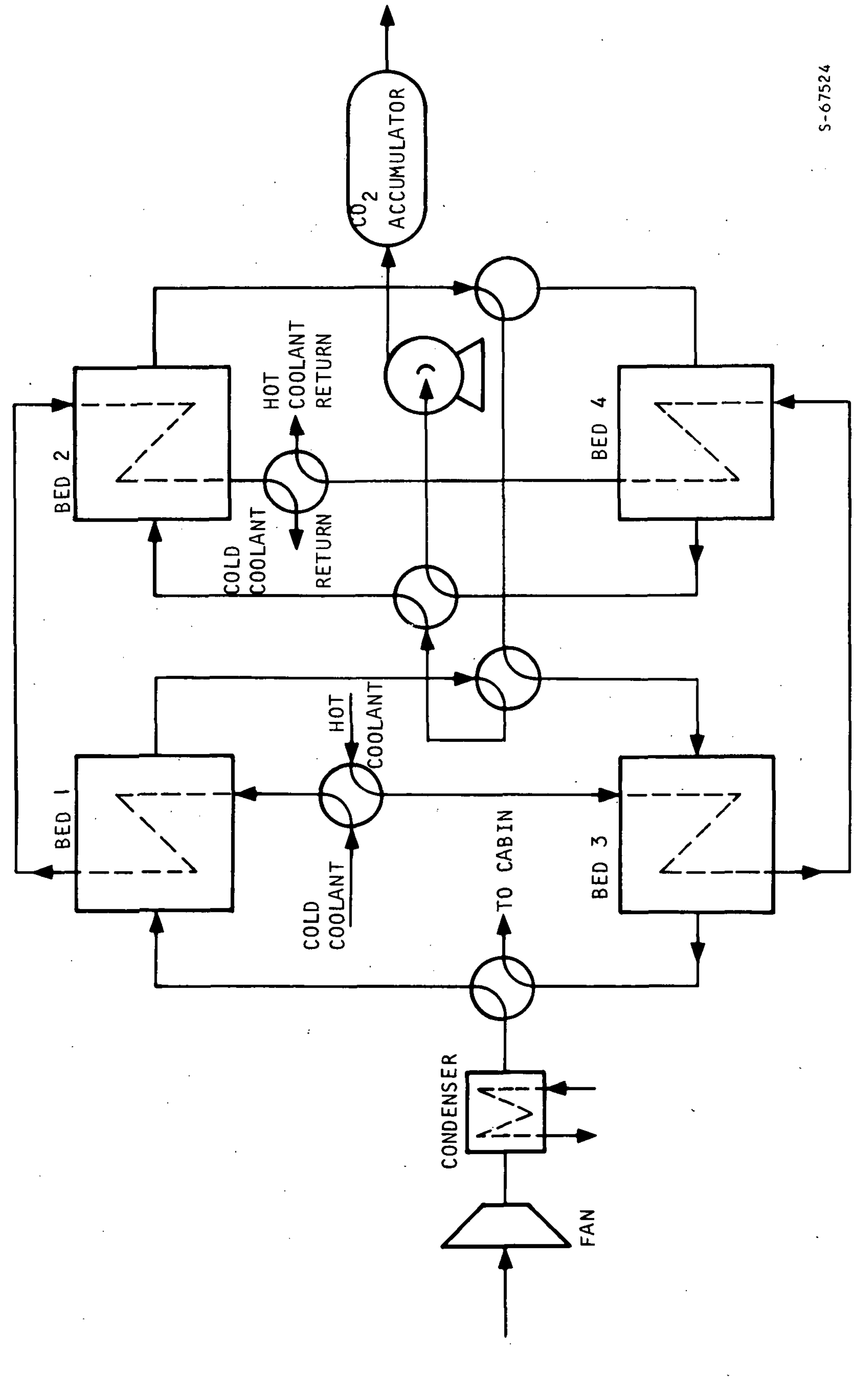

Figure 6-1. Typical 4-Bed Thermal Swing System

(c) Temperatures

(d) Sorbate loadings

(e) Average sorbate loadings

(f) Average adsorption/desorption rates

(g) Heat provided by electric heater and coolant

(h) Sorbate partial pressures

(i) Desorption pressures

(j) CO_2-accumulator pressure and volume

The bed sizes and overboard gas losses are printed again after bed sizes are adjusted to account for water poisoning effects.

PROGRAM OPTIONS

Three categories of program options are listed below.

System Options

(a) 2-bed-vacuum-dump

(b) 4-bed-H_2O-save-CO_2-dump

(c) 4-bed-H_2O-CO_2-save

Water-Poisoning Effects

(a) Degree of poisoning known

(b) Degree of poisoning to be found by the program and bed sizes adjusted accordingly

Individual Sorbent Bed Options

(a) Isothermal operation with the bed temperature specified

(b) Adiabatic operation

(c) Thermal swing operation with hot and cold coolant

(d) Thermal swing operation with an electric heater

(e) Different sorbent and bed properties for different axial nodes

(f) Desorption pressure specified as a function of time for up to three axial locations

(g) Desorption bed outlet pressure computed from vacuum duct and pump characteristics

(h) Desorption bed outlet pressure computed from input pump characteristics and CO_2 accumulator pressure.

(i) Use of a constant pressure type CO_2-accumulator

(j) Use of a constant volume type CO_2-accumulator

SECTION 7

TECHNICAL DESCRIPTION

INTRODUCTION

The technical description of program MAIN4B includes only the new features which have been added to program S9960. Basic heat and mass transfer models used in the program were described in Part I of this report.

VACUUM DUCT CHARACTERIZATION

In program S9960, an empirical correlation between duct inlet pressure and throughput was used to predict bed outlet pressures during desorption. As the correlation was based on conditions which are not universally valid, a generally applicable method was developed for the new program, MAIN4B.

In the modified analysis, the boundary condition is treated in a more general and rigorous fashion. Volumetric flow at the outlet face of the bed is calculated from pump displacement and flow conductance of the vacuum duct by

$$S = \frac{S_p C}{S_p + C} \tag{7-1}$$

where S = volumetric flow rate at the bed outlet, liters/sec

S_p = pump displacement, a function of pump inlet pressure, liters/sec

C = duct conductance, liters/sec

The duct conductance is calculated by

$$C = 3.269 \times 10^{-2} \frac{P_{av} D^4}{L\eta} + 3.81 \left(\frac{D^3}{L}\right)\left(\frac{T}{M}\right)^{\frac{1}{2}} \frac{1 + 0.147 \left(\frac{M}{T}\right)^{\frac{1}{2}} P_{av} \left(\frac{D}{\eta}\right)}{1 + 0.181 \left(\frac{M}{T}\right)^{\frac{1}{2}} P_{av} \left(\frac{D}{\eta}\right)} \tag{7-2}$$

where P_{av} = average duct pressure, torrs

D = duct diameter, cm

L = duct length, cm

M = molecular weight

T = temperature, ^{o}K

η = viscosity, poise

The characteristics of the vacuum pump used in Airlock Regenerative Carbon Dioxide Removal System qualification tests are used in the DESORB subroutine. The data statements characterizing the pump can be easily changed for different pumps. In the case of space vacuum, the pump displacements can be set to arbitrarily large quantities to simulate the almost unlimited capacity of space. The duct diameter and length set in DESØRB can also be changed for different configurations.

PUMPING INTO A CO_2-ACCUMULATOR

For a CO_2-save system, MAIN4B allows the user to specify pump characteristics in the form of displacements vs pressure ratios - VPUMP vs PUMP. The line pressure drop is neglected in this case and the boundary condition used for the bed outlet is

$$-\frac{fA}{F}\left(\frac{\partial p}{\partial X}\right) = V_p \qquad (7\text{-}3)$$

where f = void fraction

A = cross-sectional area of bed

F = bed resistance defined in Part I of this report

p = pressure, mm Hg

X = axial distance, ft

V_p = pump displacement, (cu ft)/hr

ENERGY EQUATION FOR HEAT EXCHANGER CORE METAL WITH EMBEDDED ELECTRIC HEATER

Program MAIN4B allows for the use of electric heaters embedded in heat exchanger metal. The new energy equation incorporating the heater is

$$\left(C_{px} \cdot \rho_x\right)\frac{\partial T_x}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial T_x}{\partial x}\right) + a_{vx} \cdot \left[h_{xs}\left(T_s - T_x\right) + h_{xg}\left(T_g - T_x\right) + h_{xc}\left(T_c - T_x\right)\right] + \dot{Q}_v \qquad (7\text{-}4)$$

where the heat source $\dot{Q}_v$ is the heater capacity in Btu/(cu ft of HX metal)

WATER POISONING OF SORBENT

Effects of the poisoning of molecular sieve sorbents 5A and 13X by water are shown in Figures 7-1 and 7-2. These data are set up in subroutine FCØAD, in the form of H_2O loading vs CO_2 capacity as a fraction of dry sorbent capacity. Expansion of the built-in data to include coadsorption data for other sorbents can be easily done whenever such data become available.

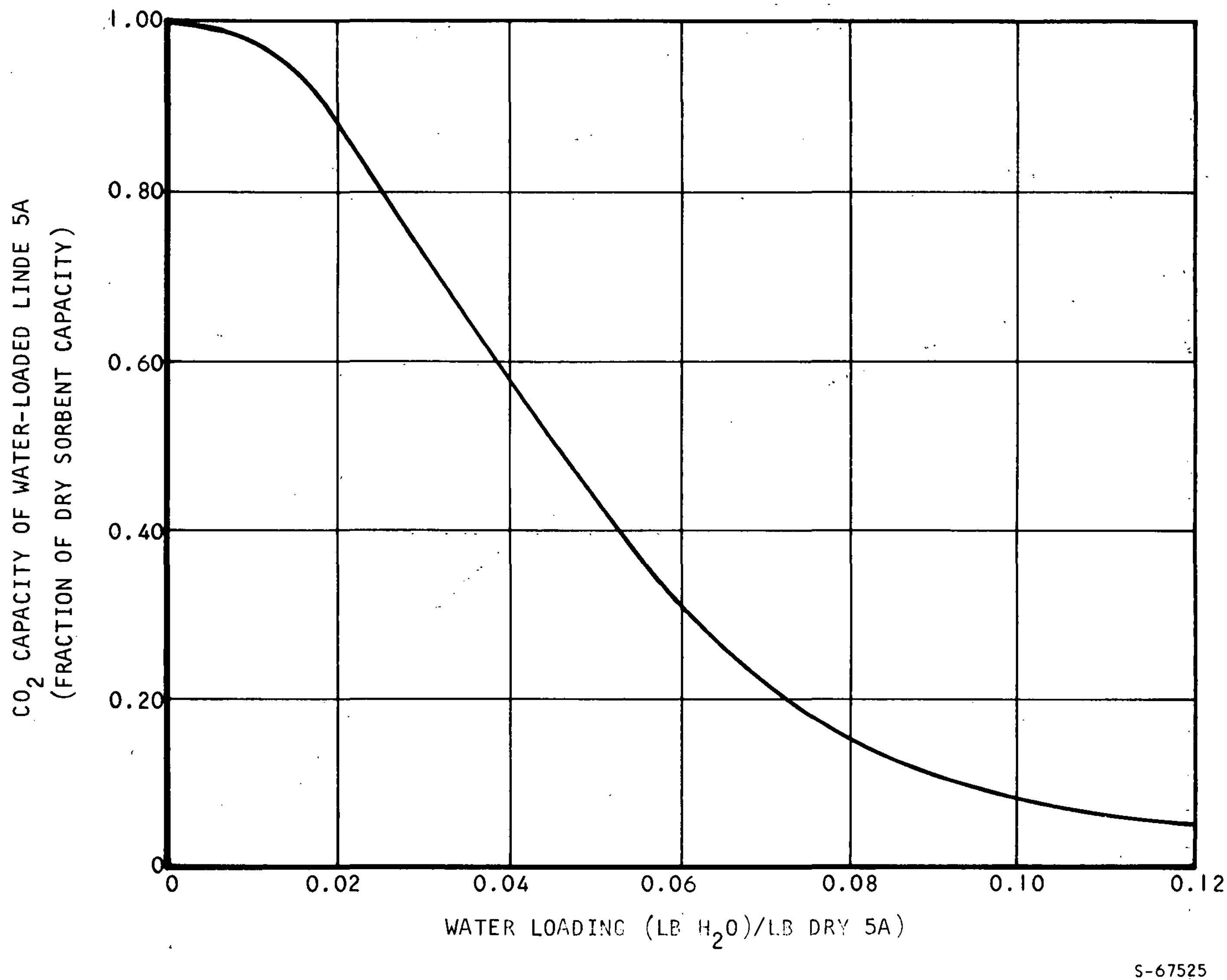

Figure 7-1. Effect of Water Poisoning on Linde 5A Capacity for CO_2

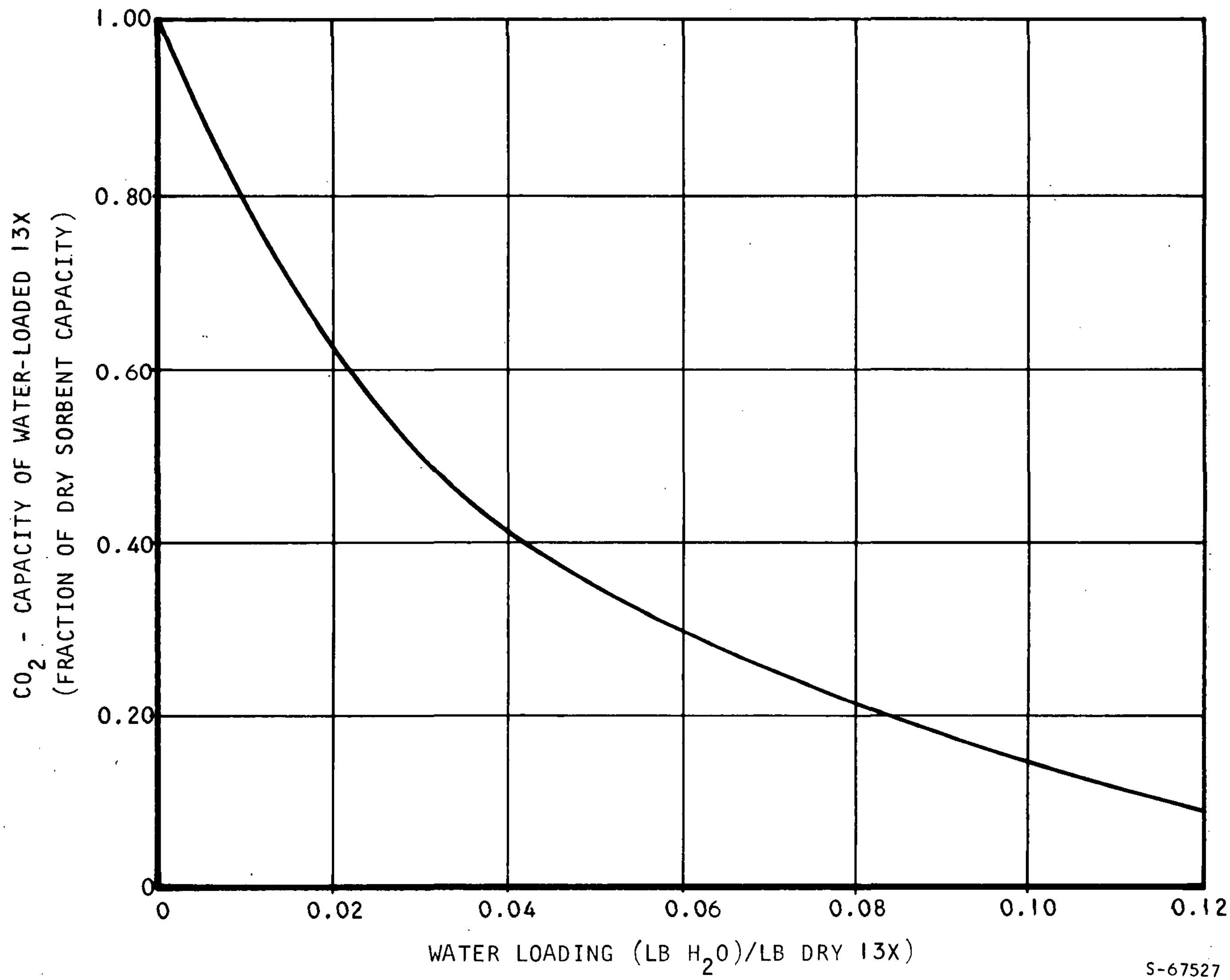

Figure 7-2. Effect of Water Poisoning on Linde 13X Capacity for CO_2

OVERBOARD GAS LOSSES

Overboard gas losses are estimated by assuming that, for molecular sieve sorbents 5A and 13X, the percentage reduction in capacity due to water poisoning is the same for CO_2, N_2 and O_2.

MAIN PROGRAM MAIN4B

The main program MAIN4B was written for a typical CO_2-H_2O-save thermal swing 4-bed system, depicted in Figure 6-1. A logic diagram of the program is shown in Figure 7-3. The program first determines the amount of water accumulated in each bed during the first NCT1 cycles.

In the input data, NDXM and NDXMAC for each bed are selected so that the CO_2 sorbent nodes which may potentially be poisoned in NCT1 cycles are assigned as desiccant nodes. This results in a desiccant section greater, and a CO_2-sorbent section smaller, than the actual sizes. The program is run for NCT1 cycles to let water accumulate in the back end of the desiccant section, which in actuality is the front end of the CO_2-section. This method predicts slightly less than actual performance of the CO_2-removal bed. However, in the first half of the run, i.e., for the first NCT1 cycles, only the desiccant bed performance is of primary interest, and an approximate simulation of the CO_2 bed should suffice in estimating bed poisoning.

At the end of the NCT1 cycles, during which period the accumulation of water in the front part of the CO_2-bed has been established, the effective dry sorbent quantity for CO_2 adsorption is found for each desiccant node, using the data presented in Figures 7-1 and 7-2. The total of all these equivalent dry sorbent weights is added to the CO_2-sorbent section by resetting NDXM and NDXMAC. In case a non-integral number of desiccant nodes results, desiccant densities are adjusted to keep the total weight unchanged. Mass diffusivity, mass transfer coefficient and heat of adsorption (DIF, GK, DH) for the reassigned nodes are set to those of node No. 1.

After the resetting of the beds, the program is run for additional NCT2 cycles to establish the CO_2 removal performance of the bed with the degree of poisoning established in the first stage of the run. NCT2 is selected just large enough to give a stabilized solution.

In Figure 7-3, the 4-bed performance prediction is performed by the operations enclosed in the broken-line rectangle, which are shown in the right hand portion of the figure.

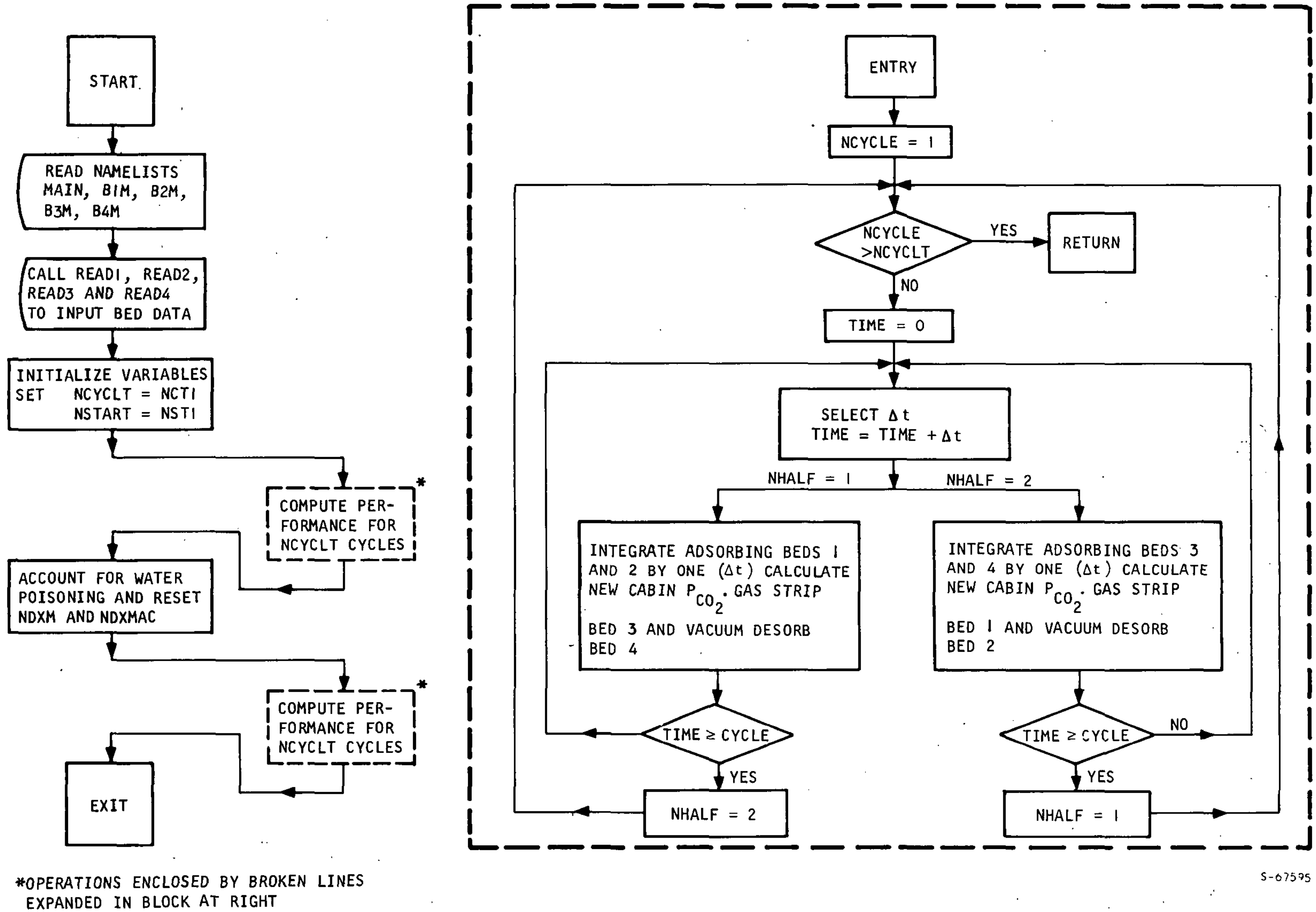

Figure 7-3. MAIN4B Program Logic

SECTION 8

USAGE

PROGRAM INPUT

All data required for program execution are inputted via eleven namelists. The following paragraphs describe the function of each namelist and define parameters/variables in the namelists.

Function of Various Namelists

Parameters defining the system and execution mode, common to all the beds, are contained in the namelist 'MAIN'. These include, among others, molecular weights of sorbates, half-cycle time, CO_2-accumulator volume, and number of cycles to be run before the effect of water-poisoning will be evaluated.

Initial conditions, gas flow rates, P_{N_2} and P_{O_2} for each bed are included in namelists 'B1M', 'B2M', B3M', and 'B4M', respectively.

Desiccant bed characteristics, such as bed and sorbent sizes, various areas, sorbent-type used for each node, desorption mode to be used, etc., make up the namelist 'DB'.

Data characterizing desiccant bed mass and heat transfer processes, are included in 'DBA' for the adsorption half-cycle and 'DBD' for the desorption half-cycle.

Similarly, corresponding data for the molecular sieve beds are contained in the namelists 'MB', 'MBA' and 'MBD'

Input Variable Lists and Definition

1. Namelist MAIN

Fortran Symbol	Definition
WM(2)	Adsorbate molecular weight; eg., WM(1) = (CO_2), WM(2) = 18 (H_2O)
CYCLE	Cycle time per one adsorption or one desorption, period, hr
DTMAX	Maximum allowable time step size, usually 0.01 hr for isothermal analysis and 0.005 hr for nonisothermal analysis
WI	Maximum loading change allowable per time increment in selecting Δt, lb/lb

TI	Maximum temperature change allowable per time increment in selecting Δt, ^oF
PCØ2C	Initial CO_2 partial pressure in cabin, mm Hg
VØLCAB	Cabin volume for atmosphere, cu ft; use VØLCAB = 10^{20}, for constant PCØ2C
RCØ2C	Rate of CO_2 generation in cabin, lb CO_2 per hr
NPRINT	Integer control variable which determines frequency of printout occurrence; e.g., if NPRINT - 2, printout occurs after every two time steps
NDTCØN	If NDTCØN = 1, Δt will be selected such that ΔT = TI, ΔW = WI for time step; if NDTCØN = 2, ΔT's as set in program will be used
NTEMP	Integer control variable; if NTEMP = 0, isothermal analysis; the energy equations are ignored, and the bed temperature is set equal to TCIN. If NTEMP $\neq$ 0, nonisothermal analysis
TGC	Cabin temperature, ^oF
PAC	Cabin pressure, mm Hg
PH2ØC	Cabin P_{H_2O}, mm Hg
TGHX	Maximum temperature allowable for CO_2-beds inlet gas, if the temperature is exceeded, a gas cooler will be employed to lower the temperature to TGHX.
PCØ2A	CO_2 accumulator pressure, for a fixed volume type, psia
VCØ2A	CO_2 accumulator volume for a fixed pressure type, cu ft
SABCØ2	CO_2 flow-rate to Sabatier reactor, lb CO_2/hr.
TCØ2A	CO_2 accumulator temperature, ^oF

KBED(4)	Index indicating whether a bed exists. E.g., if only bed 2 exists, KBED = 0, 1, 0, 0
TIMEDS	If TIMEDS<CYCLE, heat is available only during TIMEDS of the desorption half-cycle, beyond TIMEDS hot coolant, electric heater will be shut off.
NCT1	Total number of complete adsorption-desorption cycle calculations desired before effects of bed-poisoning will be assessed and bed sized adjusted accordingly to predict bed performance.
NST1	Cycle at which print-out will be started for the aforementioned run.
NCT2	Total number of complete adsorption-desorption cycle calculations desired after bed adjustments for poisoning.
NST2	Cycle at which print-out will be started for the run with adjustments for poisoning.

2. Namelist B1M

Fortran Symbol	Definition
PA1	Bed No. 1 total pressure, mm Hg
TS01(20)	Bed No. 1 initial sorbent temperature, ^{o}F
TC01(20)	Bed No. 1 initial coolant temperature, ^{o}F
TX01(20)	Bed No. 1 initial HX metal temperature, ^{o}F
W1 (4,20)	Bed No. 1 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes; 2nd subscript denoting axial nodes; lb sorbate/lb dry sorbent.
GMR1	Bed No. 1 process gas flow rate, lb/hr
GMW1	Bed No. 1 process gas molecular weight
PN21	Bed No. 1 N_2 partial pressure, mm Hg
PØ21	Bed No. 1 O_2 partial pressure, mm Hg

3. Namelist B2M

Fortran Symbol	Definition
PA2	Bed No. 2 total pressure, mm Hg
TS02(20)	Bed No. 2 initial sorbent temperature, ^oF
TC02(20)	Bed No. 2 initial coolant temperature, ^oF
TX02(20)	Bed No. 2 initial HX metal temperature, ^oF
W2(4,20)	Bed No. 2 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes; 2nd subscript denoting axial nodes; lb sorbate/lb dry sorbent.
GMR2	Bed No. 2 process gas flow rate, lb/hr
GMW2	Bed No. 2 process gas molecular weight
PN22	Bed No. 2 N_2 partial pressure, mm Hg
PØ22	Bed No. 2 O_2 partial pressure, mm Hg

4. Namelist B3M

Fortran Symbol	Definition
PA3	Bed No. 3 total pressure, mm Hg
TS03	Bed No. 3 initial sorbent temperature, ^oF
TC03	Bed No. 3 initial coolant temperature, ^oF
TX03	Bed No. 3 initial HX metal temperature, ^oF
W3	Bed No. 3 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes, 2nd subscript denoting axial nodes, lb sorbate/lb dry sorbent.
GMR3	Bed No. 3 process gas flow rate, lb/hr.
GMW3	Bed No. 3 process gas molecular weight.
PN23	Bed No. 3 N_2 partial pressure, mm Hg.
PØ23	Bed No. 3 O_2 partial pressure, mm Hg.

5. Namelist B4M

Fortran Symbol	Definition
PA4	Bed No. 4 adsorption cycle total pressure, mm Hg
TS04	Bed No. 4 initial sorbent temperature, ^{o}F
TC04	Bed No. 4 initial coolant temperature, ^{o}F
TX04	Bed No. 4 initial HX metal temperature, ^{o}F
W4	Bed No. 4 initial sorbate loading, 1st subscript denoting sorbent interior radial nodes, 2nd subscript denoting axial nodes; lb sorbate/lb dry sorbent.
GMR4	Bed No. 4 process gas flow rate, lb/hr.
GMW4	Bed No. 4 process gas molecular weight.
PN24	Bed No. 4 adsorption cycle N_2 partial pressure, mm Hg.
PØ24	Bed No. 4 adsorption cycle O_2 partial pressure, mm Hg.

6. Namelist DB

Fortran Symbol	Definition
ABED (20)	Sorbent bed cross-section area normal to flow of process gas, sq ft
AVC (20)	Primary heat exchanger plate area per unit volume of coolant held up in HX, sq ft/(cu ft)
ASX (20)	Heat exchanger primary area per unit volume sorbent bed, sq ft/(cu ft)
AGX (20)	Identical to ASX
AVX (20)	Primary heat exchanger plate area per unit volume of heat exchanger core metal, sq ft/(cu ft)
RHØG (20)	Gas density, lb/(cu ft)

RHØSB (20)	Sorbent bulk density, lb/(cu ft)
RHØS (20)	Sorbent particle density, lb/(cu ft)
RHØC (20)	Coolant density, lb/(cu ft)
RHØX (20)	Heat exchanger metal density, lb/(cu ft)
CPG (20)	Specific heat of the process gas, Btu/(lb)(^{o}F)
CPC (20)	Coolant specific heat, Btu/(lb) (^{o}F)
CPX (20)	Heat exchanger specific heat, Btu/(^{o}F)(lb)
CPP (20)	Specific heat of dry sorbent, Btu/(lb)(^{o}F)
DX	Axial node dimension, ft
NPSET(3)	Denotes nodes to which vacuum is applied
NDR4	Integer denoting total number of radial sorbent pellet nodes (interior nodes)
NDXMAC	Integer denoting number of active molecular sieve nodes, i.e., (NDXM - NDXMAC) represents the number of molecular sieve nodes which have been inactivated by water poisoning
NBCØUT	Integer control variable; NBCØUT = 1, vacuum duct is simulated; NBCØUT = 2, pressures are set as functions of time at nodes NPSET(1~3); NBCØUT = 3, 4, CO_2 save system with pump characteristics inputted; fixed volume CO_2-accumulator used for NBCØUT =3,fixed pressure accumulator for NBCØUT = 4
NDXI	Integer denoting total number of axial nodes
NDXM	Integer denoting total number of modecular sieve nodes
NØG	Node to which coolant is added
PØUT (10) TIMET (10)	10 pairs of exit pressure vs time data to be used if NBCOUT = 2; POUT = vacuum end manifold pressures (mm Hg), TIMET = times (hr)

PUMP (10) VPUMP (10)	10 pairs of pressure ratios vs volumetric displacements to be used for NBCØUT = 3 or 4; PUMP = pump outlet to pump inlet pressure ratio; VPUMP = volumetric displacements, cfm.
IDSØRB (20)	Index identifying sorbent used for each node; 1 = 5A, 2 = S.G., 3 = 13X, 4 = 4A, 5 = 3A.
CPL (2)	Specific heat of adsorbed sorbate, Btu/ (°F) (lb)
DP (20)	Sorbent diameter, ft.

7. Namelist DBA

Fortran Symbol	Definition
HXG (20)	Heat transfer coefficient, heat exchanger to process gas, Btu/(sq ft) (°F) (hr)
HXS (20)	Heat transfer coefficient, heat exchanger to sorbent, Btu/(sq ft)(hr)(°F)
HXC (20)	Heat transfer coefficient, heat exchanger to coolant Btu/(sq ft)(hr)(°F)
HSG (20)	Heat transfer coefficient, sorbent to gas, Btu/(hr)(sq ft)(°F)
SK (20)	Effective sorbent thermal conductivity, Btu/(hr) (sq ft) (°F/ft)
TKX (20)	Heat exchanger metal thermal conductivity, TKX (K) denotes that between node K-1 and node K, Btu/(hr)(sq ft)(°F/ft)
DH (20)	Differential heat of adsorption, Btu/(lb adsorbed)
DIF (20)	Internal diffusivity, sq ft/hr
GK (20)	External surface mass transfer coefficient, lb-mol/(hr)(sq ft)(mm Hg)
TCIN	Coolant inlet temperature, °F
HTR (20)	Electric heater power for each node, BTU/hr

TMAX — Maximum metal temperature, above which heater will be shut off, ^{0}F.

WC — Coolant flow rate, lb/hr.

8. Namelist DBD

Parameters characterizing various transfer processes in desorption cycles are contained in this namelist. The list is identical to DBA and will be given below without definition.

HXG (20), HXS(20), HXC(20), HSG(20), SK (20), TKX (20), DH (20), DIF (20), GK (20), TCIN, HTR (20), TMAX, WC

9. Namelist MB

This namelist comprises the characteristics of CO_2 beds 2 and 4. The list is identical to DB and will be given below without definition.

ABED (20), AVC (20), ASX (20), AGX (20), AXC (20), AVX (20), RHØG (20), RHØSB (20), RHØS (20), RHØC (20), RHØX (20), GPG (20), CPC (20), CPX (20), CPP (20), DX, NPSET (3), NDR4, NDXMAC, NBCØUT, NDXI, NDXM, NØG, PØUT (10), TIMET (10), PUMP (10), VPUMP(10), IDSØRB(20), CPL (2), DP (20)

10. Namelist MBA

This namelist comprises the data characterizing various transport processes for CO_2 beds 3 and 4 adsorption cycles. The list is identical to DBA and will be given without definition.

HXG (20), HXS (20), HXC (20), HSG (20), SK (20), TKX (20), DH (20), DIF (20), GK (20), TCIN, HTR (20), TMAX, WC

11. Namelist MBD

This list is equivalent to MBA for desorption cycles.

HXG (20), HXS (20), HXC (20), HSG (20), SK (20), TKX (20), DH (20), DIF (20), GK (20), TCIN, HTR (20), TMAX, WC

EXECUTION CHARACTERISTICS

Storage Requirement

The present program requires a 28,400 word storage on the Univac 1108 computer.

Execution Time

With the Univac 1108 computer and using a total of 20 nodes for all four beds, the ratio of real time to computer time is roughly 130 to 1.

Accuracy/Validity

The single bed program S9960 was tested on the regenerable CO_2 removal systems for AAP and Airlock applications and has proved to be quite accurate in performance predictions. It is reasonable to assume that the expanded version, MAIN4B, should be able to predict the performance of a 4-bed-CO_2-H_2O-save system equally well, as the basic models employed in both programs are identical.

Program Limitations

Although the present program was intended to be as general as feasible, the basic system configuration as shown in Figure 6-1 was assumed in writing the main program MAIN4B. Should the coolant hook-up be different from the arrangement depicted in the schematic, the main program must be modified. The work involved should be minimal, however.

Another limitation is that the program uses the built-in equilibrium data of subroutine EQPWT, which represents the best data available at AiResearch at the moment. As better data become available, the subroutine has to be modified. Also pure N_2 and pure O_2 data are employed by the program in estimating overboard gas losses. Should expanded N_2 - O_2 coadsorption data become available, some modifications will be required in the estimation.

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SECTION 9

EXAMPLE RUNS

INTRODUCTION

Two example runs are presented in this section: a performance prediction for a 4-bed-CO_2-H_2O save system; and demonstration of the program to account for the coadsorption of CO_2 with H_2O. Program input and output data are included.

Example run no. 1 is presented on page 144 and example run no. 2 is presented on page 165.

EXAMPLE RUN NO. 1

EXAMPLE RUN NO. 1

The first example to be presented is the performance prediction for a 4-bed-CO_2-H_2O save system. This example is very similar to the one shown in Figure 6-1, except that temperature swings of the CO_2 beds are controlled electrically, and an intercooler is used to precool the CO_2-bed inlet gas stream to 50^oF.

Input data required are given as Figure 9-1. These data are printed by the program in the namelist format for input data checking. It should be noted that since no coolant is used in the sorbent beds of the present system, coolant-related data are unimportant for the run. As vacuum dumping is not used for sorbent regeneration, there should be no overboard gas losses, and so PN21, PO21, PN22, PO22, etc., are set to 10^{-20}. (Setting these to zero causes some problems.)

After the printing of the input data, the program then gives sorbent quantities and estimated gas losses for each bed, as shown in Figure 9-2.

The program is run with NCT1=6 and NST1=6 and printing starts at the 6th cycle. The print-out at the end of the second half of the 6th cycle is presented in Figure 9-3 for all four beds. Beds 3 and 4 have been adsorbing and beds 1 and 2 have been desorbing. A constant pressure type CO_2-accumulator is used for the system and the accumulator volume at the moment is printed with bed 2 outputs.

Since NCT2=0 for the run, the program stops at this point.

```
$MAIN
WM       =    .44000000+02,    .18000000+02,
CYCLE    =    .16000000+01,
DTMAX    =    .15000000-01,
WI       =    .49999999-02,
TI       =    .10000000+02,
PCO2C    =    .75999999+01,
VOLCAB   =    .30000000+03,
RCO2C    =    .55000000+00,
NPRINT   =             100,
NDTCON   =               1,
NTEMP    =               1,
TGC      =    .70000000+02,
PAC      =    .76000000+03,
PH2OC    =    .92000000+01,
TGHX     =    .50000000+02,
PCO2A    =    .25000000+02,
VCO2A    =    .60000000+01,
SABCO2   =    .55000000+00,
TCO2A    =    .10000000+03,
KBED     =               1,               1,               1,               1,
TIMEDS   =    .20000000+01,
NCT1     =               6,
NST1     =               6,
NCT2     =               1,
NST2     =               1,
$END
$B1M
PA1      =    .76000000+03,
TS01     =    .10000000+03,    .10000000+03,    .10000000+03,    .10000000+03,
              .10000000+03,    .10000000+03,    .10000000+03,    .10000000+03,
              .10000000+03,    .10000000+03,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TC01     =    .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TX01     =    .10000000+03,    .10000000+03,    .10000000+03,    .10000000+03,
              .10000000+03,    .10000000+03,    .10000000+03,    .10000000+03,
              .10000000+03,    .10000000+03,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
W1       =    .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
              .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
```

Figure 9-1. Input Data for Example Run No. 1

```
                 .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
                 .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
                 .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
                 .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
GMR1     =       .12500000+03,
GMW1     =       .29000000+02,
PN21     =       .10000000-19,
PO21     =       .10000000-19,
$END
$B2M
PA2      =       .76000000+03,
TS02     =       .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .00000000+00,
TC02     =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TX02     =       .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .37500000+03,
                 .37500000+03,    .37500000+03,    .37500000+03,    .00000000+00,
W2       =       .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
                 .10000000-01,    .10000000-01,    .10000000-01,    .10000000-01,
GMR2     =       .12500000+03,
GMW2     =       .29000000+02,
PN22     =       .10000000-19,
PO22     =       .10000000-19,
$END
$B3M
PA3      =       .76000000+03,
TS03     =       .10000000+03,    .10000000+03,    .10000000+03,    .10000000+03,
                 .10000000+03,    .10000000+03,    .10000000+03,    .10000000+03,
                 .10000000+03,    .10000000+03,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TC03     =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                 .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
```

Figure 9-1. (Continued)

```
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
TX03       =      .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
W3         =      .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
                  .69999998-01,     .69999998-01,     .69999998-01,     .69999998-01,
GMR3       =      .12500000+03,
GMW3       =      .29000000+02,
PN23       =      .10000000-19,
PO23       =      .10000000-19,
$END
$B4M
PA4        =      .76000000+03,
TS04       =      .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .00000000+00,
TC04       =      .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
TX04       =      .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .10000000+03,
                  .10000000+03,     .10000000+03,     .10000000+03,     .00000000+00,
W4         =      .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
                  .10000000-01,     .10000000-01,     .10000000-01,     .10000000-01,
```

Figure 9-1. (Continued)

```
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
          .10000000-01,   .10000000-01,   .10000000-01,   .10000000-01,
GMR4    = .12500000+03,
GMW4    = .29000000+02,
PN24    = .10000000-19,
PO24    = .10000000-19,
$END
$DB
ABED    = .10000000+01,   .10000000+01,   .10000000+01,   .10000000+01,
          .10000000+01,   .10000000+01,   .10000000+01,   .10000000+01,
          .10000000+01,   .10000000+01,   .10000000+01,   .10000000+01,
          .10000000+01,   .10000000+01,   .10000000+01,   .10000000+01,
          .10000000+01,   .10000000+01,   .10000000+01,   .10000000+01,
AVC     = .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
ASX     = .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
AGX     = .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
AVX     = .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
RHOG    = .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
RHOSB   = .45000000+02,   .45000000+02,   .45000000+02,   .45000000+02,
          .45000000+02,   .45000000+02,   .45000000+02,   .45000000+02,
          .45000000+02,   .45000000+02,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
RHOS    = .64000000+02,   .64000000+02,   .64000000+02,   .64000000+02,
          .64000000+02,   .64000000+02,   .64000000+02,   .64000000+02,
          .64000000+02,   .64000000+02,   .64000000+02,   .64000000+02,
          .64000000+02,   .64000000+02,   .64000000+02,   .64000000+02,
          .64000000+02,   .64000000+02,   .64000000+02,   .64000000+02,
RHOC    = .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
          .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
```

Figure 9-1. (Continued)

```
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
 RHOX     =     .49000000+03,     .49000000+03,     .49000000+03,     .49000000+03,
                .49000000+03,     .49000000+03,     .49000000+03,     .49000000+03,
                .49000000+03,     .49000000+03,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
 CPG      =     .23000000+00,     .23000000+00,     .23000000+00,     .23000000+00,
                .23000000+00,     .23000000+00,     .23000000+00,     .23000000+00,
                .23000000+00,     .23000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
 CPC      =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
 CPX      =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
 CPP      =     .25000000+00,     .25000000+00,     .25000000+00,     .25000000+00,
                .25000000+00,     .25000000+00,     .25000000+00,     .25000000+00,
                .25000000+00,     .25000000+00,     .25000000+00,     .25000000+00,
                .25000000+00,     .25000000+00,     .25000000+00,     .25000000+00,
                .25000000+00,     .25000000+00,     .25000000+00,     .25000000+00,
 DX       =     .25000000+00,
 NPSET    =                 ,                 ,                 ,
 NDR4     =                2,
 NDXMAC   =                 ,
 NBCOUT   =                 ,
 NDX1     =                5,
 NDXM     =                 ,
 NOG      =                1,
 POUT     =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,
 TIMET    =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,
 PUMP     =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,
 VPUMP    =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                .00000000+00,     .00000000+00,
 IDSORB   =                3,                3,                3,                3,
                           3,                3,                3,                3,
                           3,                3,                3,                3,
                           3,                3,                3,                3,
                           3,                3,                3,                3,
 CPL      =     .10200000+01,     .10000000+01,
 DP       =     .64199999-02,     .64199999-02,     .64199999-02,     .64199999-02,
                .64199999-02,     .64199999-02,     .64199999-02,     .64199999-02,
                .64199999-02,     .64199999-02,     .64199999-02,     .64199999-02,
                .64199999-02,     .64199999-02,     .64199999-02,     .64199999-02,
                .64199999-02,     .64199999-02,     .64199999-02,     .64199999-02,
 $END
 $DBA
 HXG      =     .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
```

Figure 9-1. (Continued)

```
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
HXS     =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
HXC     =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
HSG     =       .20000000+02,    .20000000+02,    .20000000+02,    .20000000+02,
                .20000000+02,    .20000000+02,    .20000000+02,    .20000000+02,
                .20000000+02,    .20000000+02,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
SK      =       .00000000+00,    .99999998-01,    .99999998-01,    .99999998-01,
                .99999998-01,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TKX     =       .00000000+00,    .90000000+01,    .90000000+01,    .90000000+01,
                .90000000+01,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
DH      =       .14000000+04,    .14000000+04,    .14000000+04,    .14000000+04,
                .14000000+04,    .14000000+04,    .14000000+04,    .14000000+04,
                .14000000+04,    .14000000+04,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
DIF     =       .40000000-03,    .40000000-03,    .40000000-03,    .40000000-03,
                .40000000-03,    .40000000-03,    .40000000-03,    .40000000-03,
                .40000000-03,    .40000000-03,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
GK      =       .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
TCIN    =       .00000000+00,
HTR1    =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TMAX    =       .40000000+03,
WCC     =       .00000000+00,
$END
$DBD
HXG     =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
                .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
HXS     =       .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
```

Figure 9-1. (Continued)

```
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
HXC      =     .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
HSG      =     .20000000+02,  .20000000+02,  .20000000+02,  .20000000+02,
               .20000000+02,  .20000000+02,  .20000000+02,  .20000000+02,
               .20000000+02,  .20000000+02,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
SK       =     .00000000+00,  .99999998-01,  .99999998-01,  .99999998-01,
               .99999998-01,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
TKX      =     .00000000+00,  .90000000+01,  .90000000+01,  .90000000+01,
               .90000000+01,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
DH       =     .14000000+04,  .14000000+04,  .14000000+04,  .14000000+04,
               .14000000+04,  .14000000+04,  .14000000+04,  .14000000+04,
               .14000000+04,  .14000000+04,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
DIF      =     .40000000-03,  .40000000-03,  .40000000-03,  .40000000-03,
               .40000000-03,  .40000000-03,  .40000000-03,  .40000000-03,
               .40000000-03,  .40000000-03,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
GK       =     .10000000-02,  .10000000-02,  .10000000-02,  .10000000-02,
               .10000000-02,  .10000000-02,  .10000000-02,  .10000000-02,
               .10000000-02,  .10000000-02,  .10000000-02,  .10000000-02,
               .10000000-02,  .10000000-02,  .10000000-02,  .10000000-02,
               .10000000-02,  .10000000-02,  .10000000-02,  .10000000-02,
TCIN     =     .00000000+00,
HTR1     =     .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
TMAX     =     .40000000+03,
WCC      =     .00000000+00,
$END
$MB
ABED     =     .79999999+00,  .79999999+00,  .79999999+00,  .79999999+00,
               .79999999+00,  .79999999+00,  .79999999+00,  .79999999+00,
               .79999999+00,  .79999999+00,  .79999999+00,  .79999999+00,
               .79999999+00,  .79999999+00,  .79999999+00,  .79999999+00,
               .79999999+00,  .79999999+00,  .79999999+00,  .79999999+00,
AVC      =     .52100000+03,  .52100000+03,  .52100000+03,  .52100000+03,
               .52100000+03,  .52100000+03,  .52100000+03,  .52100000+03,
               .52100000+03,  .52100000+03,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
               .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
ASX      =     .40000000+02,  .40000000+02,  .40000000+02,  .40000000+02,
```

Figure 9-1. (Continued)

```
                .40000000+02,  .40000000+02,  .40000000+02,  .40000000+02,
                .40000000+02,  .40000000+02,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
AGX      =      .16000000+02,  .16000000+02,  .16000000+02,  .16000000+02,
                .16000000+02,  .16000000+02,  .16000000+02,  .16000000+02,
                .16000000+02,  .16000000+02,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
AVX      =      .32800000+03,  .32800000+03,  .32800000+03,  .32800000+03,
                .32800000+03,  .32800000+03,  .32800000+03,  .32800000+03,
                .32800000+03,  .32800000+03,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
RHOG     =      .30000000-03,  .30000000-03,  .30000000-03,  .30000000-03,
                .30000000-03,  .30000000-03,  .30000000-03,  .30000000-03,
                .30000000-03,  .30000000-03,  .30000000-03,  .30000000-03,
                .30000000-03,  .30000000-03,  .30000000-03,  .30000000-03,
                .30000000-03,  .30000000-03,  .30000000-03,  .30000000-03,
RHOSB    =      .37000000+02,  .37000000+02,  .37000000+02,  .37000000+02,
                .37000000+02,  .37000000+02,  .37000000+02,  .37000000+02,
                .37000000+02,  .37000000+02,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
RHOS     =      .64000000+02,  .64000000+02,  .64000000+02,  .64000000+02,
                .64000000+02,  .64000000+02,  .64000000+02,  .64000000+02,
                .64000000+02,  .64000000+02,  .64000000+02,  .64000000+02,
                .64000000+02,  .64000000+02,  .64000000+02,  .64000000+02,
                .64000000+02,  .64000000+02,  .64000000+02,  .64000000+02,
RHOC     =      .11500000+03,  .11500000+03,  .11500000+03,  .11500000+03,
                .11500000+03,  .11500000+03,  .11500000+03,  .11500000+03,
                .11500000+03,  .11500000+03,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
RHOX     =      .49000000+03,  .49000000+03,  .49000000+03,  .49000000+03,
                .49000000+03,  .49000000+03,  .49000000+03,  .49000000+03,
                .49000000+03,  .49000000+03,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
CPG      =      .23000000+00,  .23000000+00,  .23000000+00,  .23000000+00,
                .23000000+00,  .23000000+00,  .23000000+00,  .23000000+00,
                .23000000+00,  .23000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
CPC      =      .28000000+00,  .28000000+00,  .28000000+00,  .28000000+00,
                .28000000+00,  .28000000+00,  .28000000+00,  .28000000+00,
                .28000000+00,  .28000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
CPX      =      .10999999+00,  .10999999+00,  .10999999+00,  .10999999+00,
                .10999999+00,  .10999999+00,  .10999999+00,  .10999999+00,
                .10999999+00,  .10999999+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
                .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
CPP      =      .25000000+00,  .25000000+00,  .25000000+00,  .25000000+00,
                .25000000+00,  .25000000+00,  .25000000+00,  .25000000+00,
                .25000000+00,  .25000000+00,  .25000000+00,  .25000000+00,
                .25000000+00,  .25000000+00,  .25000000+00,  .25000000+00,
                .25000000+00,  .25000000+00,  .25000000+00,  .25000000+00,
DX       =      .25000000+00,
```

Figure 9-1. (Continued)

```
NPSET   =          10,
NDR4    =           2,
NDXMAC  =           5,
NBCOUT  =           4,
NDX1    =           5,
NDXM    =           5,
NOG     =           1,
POUT    =  .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,
TIMET   =  .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,
PUMP    =  .10000000+01,  .25000000+02,  .25000000+02,  .25000000+02,
           .25000000+02,  .25000000+02,  .25000000+02,  .25000000+02,
           .25000000+02,  .25000000+02,
VPUMP   =  .30000000+01,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,
IDSORB  =             1,             1,             1,             1,
                      1,             1,             1,             1,
                      1,             1,             1,             1,
                      1,             1,             1,             1,
                      1,             1,             1,             1,
CPL     =  .10200000+01,  .10000000+01,
DP      =  .64199999-02,  .64199999-02,  .64199999-02,  .64199999-02,
           .64199999-02,  .64199999-02,  .64199999-02,  .64199999-02,
           .64199999-02,  .64199999-02,  .64199999-02,  .64199999-02,
           .64199999-02,  .64199999-02,  .64199999-02,  .64199999-02,
           .64199999-02,  .64199999-02,  .64199999-02,  .64199999-02,
$END
$MBA
HXG     =  .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
HXS     =  .96000000+01,  .96000000+01,  .96000000+01,  .96000000+01,
           .96000000+01,  .96000000+01,  .96000000+01,  .96000000+01,
           .96000000+01,  .96000000+01,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
HXC     =  .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
HSG     =  .50000000+01,  .50000000+01,  .50000000+01,  .50000000+01,
           .50000000+01,  .50000000+01,  .50000000+01,  .50000000+01,
           .50000000+01,  .50000000+01,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
SK      =  .00000000+00,  .99999998-01,  .99999998-01,  .99999998-01,
           .99999998-01,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
TKX     =  .00000000+00,  .90000000+01,  .90000000+01,  .90000000+01,
           .90000000+01,  .00000000+00,  .00000000+00,  .00000000+00,
           .00000000+00,  .00000000+00,  .00000000+00,  .00000000+00,
```

Figure 9-1. (Continued)

```
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
DH      =       .40000000+03,   .40000000+03,   .40000000+03,   .40000000+03,
                .40000000+03,   .40000000+03,   .40000000+03,   .40000000+03,
                .40000000+03,   .40000000+03,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
DIF     =       .40000000-04,   .40000000-04,   .40000000-04,   .40000000-04,
                .40000000-04,   .40000000-04,   .40000000-04,   .40000000-04,
                .40000000-04,   .40000000-04,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
GK      =       .20000000-03,   .20000000-03,   .20000000-03,   .20000000-03,
                .20000000-03,   .20000000-03,   .20000000-03,   .20000000-03,
                .20000000-03,   .20000000-03,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
TCIN    =       .00000000+00,
HTR1    =       .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
TMAX    =       .40000000+03,
WCC     =       .00000000+00,
$END
$MBD
HXG     =       .60000000+01,   .60000000+01,   .60000000+01,   .60000000+01,
                .60000000+01,   .60000000+01,   .60000000+01,   .60000000+01,
                .60000000+01,   .60000000+01,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
HXS     =       .96000000+01,   .96000000+01,   .96000000+01,   .96000000+01,
                .96000000+01,   .96000000+01,   .96000000+01,   .96000000+01,
                .96000000+01,   .96000000+01,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
HXC     =       .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
HSG     =       .50000000+01,   .50000000+01,   .50000000+01,   .50000000+01,
                .50000000+01,   .50000000+01,   .50000000+01,   .50000000+01,
                .50000000+01,   .50000000+01,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
SK      =       .00000000+00,   .99999998-01,   .99999998-01,   .99999998-01,
                .99999998-01,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
TKX     =       .00000000+00,   .90000000+01,   .90000000+01,   .90000000+01,
                .90000000+01,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
DH      =       .40000000+03,   .40000000+03,   .40000000+03,   .40000000+03,
                .40000000+03,   .40000000+03,   .40000000+03,   .40000000+03,
                .40000000+03,   .40000000+03,   .00000000+00,   .00000000+00,
```

Figure 9-1. (Continued)

```
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
DIF       =       .40000000-04,     .40000000-04,     .40000000-04,     .40000000-04,
                  .40000000-04,     .40000000-04,     .40000000-04,     .40000000-04,
                  .40000000-04,     .40000000-04,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
GK        =       .20000000-03,     .20000000-03,     .20000000-03,     .20000000-03,
                  .20000000-03,     .20000000-03,     .20000000-03,     .20000000-03,
                  .20000000-03,     .20000000-03,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                  .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
TCIN      =       .00000000+00,
HTR1      =       .10000000+04,     .10000000+04,     .10000000+04,     .10000000+04,
                  .10000000+04,     .10000000+04,     .10000000+04,     .10000000+04,
                  .10000000+04,     .10000000+04,     .10000000+04,     .10000000+04,
                  .10000000+04,     .10000000+04,     .10000000+04,     .10000000+04,
                  .10000000+04,     .10000000+04,     .10000000+04,     .10000000+04,
TMAX      =       .40000000+03,
WCC       =       .00000000+00,
$END
```

Figure 9-1. (Continued)

BED NO 1

VOLUME AND WEIGHT

BULK VOLUME OF CO2 SORBENT (CU FT)	.0000
WEIGHT OF CO2 SORBENT (LB)	.0000
WEIGHT OF ACTIVE CO2 SORBENT (LB)	.0000
BULK VOLUME OF DESICCANT (CU FT)	1.2500
WEIGHT OF DESICCANT (LB)	56.2500

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. Sorbent Bed Size and Gas Loss

BED NO 2

VOLUME AND WEIGHT

BULK VOLUME OF CO2 SORBENT (CU FT)	1.0000
WEIGHT OF CO2 SORBENT (LB)	37.0000
WEIGHT OF ACTIVE CO2 SORBENT (LB)	37.0000
BULK VOLUME OF DESICCANT (CU FT)	.0000
WEIGHT OF DESICCANT (LB)	.0000

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. (Continued)

BED NO 3

VOLUME AND WEIGHT

BULK VOLUME OF CO2 SORBENT (CU FT)	.0000
WEIGHT OF CO2 SORBENT (LB)	.0000
WEIGHT OF ACTIVE CO2 SORBENT (LB)	.0000
BULK VOLUME OF DESICCANT (CU FT)	1.2500
WEIGHT OF DESICCANT (LB)	56.2500

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. (Continued)

BED NO 4

VOLUME AND WEIGHT

BULK VOLUME OF CO2 SORBENT (CU FT)	1.0000
WEIGHT OF CO2 SORBENT (LB)	37.0000
WEIGHT OF ACTIVE CO2 SORBENT (LB)	37.0000
BULK VOLUME OF DESICCANT (CU FT)	.0000
WEIGHT OF DESICCANT (LB)	.0000

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0000
OXYGEN LOSS (LB/HR)	.0000

Figure 9-2. (Continued)

```
BED NO.  3

ADSORPTION CYCLE  6
  TIME=  1.60000 HR       96.000 MIN     TIME INCREMENT= .01302 HR
```

AXIAL NODE	PCO2,MM	PH2C,MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	2.5782	.0000	112.9449	112.8917	-.0000	-.0000
2	2.5782	.0003	119.0301	119.0147	-.0000	-.0000
3	2.5782	.0077	120.7881	120.8000	-.0000	-.0000
4	2.5782	.2311	119.4347	119.6553	-.0000	-.0000
5	2.5782	5.1786	94.2263	94.4383	.0000	.0000
INLET	2.5782	9.2000	70.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB

AXIAL NODE \ SORB NODE	AVG	1	2	3	4
1	.0267	.0267	.0267		
2	.0333	.0333	.0333		
3	.0389	.0389	.0389		
4	.0888	.0887	.0890		
5	.2153	.2152	.2154		

```
AVG CO2 LOADING IN CO2 SORBENT (LB/LB)   @@@@@@@@@@@@     .0000
TIME AVG CO2 ADSORPTION RATE (LB/HR)     @@@@@@@@@@@@     .0000
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)@@@@@@     .0000
TIME AVG OUTLET PH2O (MM)   @@@@@@@@@@@@@@@@@@@@@@@@      .0000

AVG H2O LOADING IN DESICCANT (LB/LB)       @@@@@@@@@@@@    .0806
TIME AVG H2O ADSORPTION RATE (LB/HR)       @@@@@@@@@@@@    .9392
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)@@@@@@     -.0000
```

Figure 9-3. Print-Out at End of Six Complete Cycles

BED NO. 4

ADSORPTION CYCLE 6
TIME= 1.60000 HR 96.000 MIN TIME INCREMENT= .01302 HR

AXIAL NODE	PCO2,MM	PH2O,MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	.4373	.0000	60.5864	60.7142	-.0000	60.8095
2	.8735	.0000	58.1843	58.3396	-.0000	58.4635
3	1.4763	.0000	55.2669	55.4178	-.0000	55.5300
4	2.0998	.0000	52.4302	52.5273	-.0000	52.6288
5	2.4923	.0000	50.6068	50.6391	.0000	50.7356
INLET	2.5782	.0000	50.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB NODE / AXIAL NODE	AVG	1	2	3	4
1	.0120	.0115	.0125		
2	.0210	.0203	.0217		
3	.0334	.0327	.0341		
4	.0454	.0450	.0459		
5	.0540	.0539	.0541		

AVG CO2 LOADING IN CO2 SORBENT (LB/LB) @@@@@@@@@@@@ .0332
TIME AVG CO2 ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ .5501
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)@@@@@@ .0000
TIME AVG OUTLET PH2O (MM) @@@@@@@@@@@@@@@@@@@@@@@@ .0000

AVG H2O LOADING IN DESICCANT (LB/LB) @@@@@@@@@@@@ .0000
TIME AVG H2O ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ .0000
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)@@@@@@ -.0000

Figure 9-3. (Continued)

BED NO. 1

ADSORPTION CYCLE 6
TIME= 1.60000 HR 96.000 MIN TIME INCREMENT= .01302 HR

AXIAL NODE	PCO2,MM	PH2O,MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	.4373	.0000	61.7283	61.7383	.0000	.0000
2	.4373	.0000	65.1308	65.1606	-.0000	-.0000
3	.4373	.0000	67.7681	67.7912	-.0000	-.0000
4	.4373	.0000	49.6426	49.4840	-.0000	-.0000
5	.4373	.0013	31.4529	31.2937	-.0000	-.0000
INLET	.4373	.0000	60.5864			

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB NODE / AXIAL NODE	AVG	1	2	3	4
1	.0263	.0263	.0263		
2	.0329	.0329	.0329		
3	.0375	.0375	.0375		
4	.0624	.0624	.0624		
5	.1114	.1114	.1114		

AVG CO2 LOADING IN CO2 SORBENT (LB/LB) @@@@@@@@@@@@ .0000
TIME AVG CO2 ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ .0000
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)@@@@@@ .0000
TIME AVG OUTLET PH2O (MM) @@@@@@@@@@@@@@@@@@@@@@@@ 10.2134

AVG H2O LOADING IN DESICCANT (LB/LB) @@@@@@@@@@@@ .0541
TIME AVG H2O ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ -1.0427
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)@@@@@@ -.0000

Figure 9-3. (Continued)

BED NO. 2

DESORPTION CYCLE 6
TIME= 1.60000 HR 96.000 MIN TIME INCREMENT= .01302 HR

AXIAL NODE	TOTAL PRESS,MM	GAS TEMP,DEG F	SORBENT TEMP, DEG F	COOLANT TEMP,DEG F	HX CORE TEMP, DEG F
1	54.2657	390.8997	390.8997	-.0000	391.1669
2	54.2541	405.1958	405.2043	-.0000	404.9627
3	54.2338	404.0395	404.0437	-.0000	403.9226
4	54.2042	395.7084	395.7072	-.0000	395.7357
5	54.1641	389.0017	388.9976	.0000	389.1141

LOADING AT INTERIOR OF SORBENT

SORB NODE / AXIAL NODE	AVG	1	2	3	4
1	.0095	.0096	.0094		
2	.0092	.0093	.0092		
3	.0093	.0094	.0092		
4	.0094	.0095	.0093		
5	.0095	.0096	.0094		

AVG CO2 LOADING IN CO2 SORBENT (LB/LB) @@@@@@@@@@@@ .0094
TIME AVG CO2 DESORPTION RATE (LB/HR) @@@@@@@@@@@@ .5505
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)@@@@@@ 2.1730
ACCUMULATOR CO2 PRESSURE (PSIA) @@@@@@@@@@@@@@@@@@ 25.0000

AVG H2O LOADING IN DESICCANT (LB/LB) @@@@@@@@@@@@ .0000
TIME AVG H2O ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ -.0000
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)@@@@@@ -.0000
CO2 ACCUMULATOR VOLUME (CU FT) @@@@@@@@@@@@@@@@@@ 2.6784

Figure 9-3. (Continued)

EXAMPLE RUN NO. 2

EXAMPLE RUN NO. 2

In the second example, the capability of the program to account for the coadsorption of CO_2 with H_2O is demonstrated. To utilize this capability, the program must be run in two stages. In the first stage, the program is run for NCT1 cycles to establish the amount of water accumulated in a sorbent bed after NCT1 cycles of operation. The quantity of CO_2-sorbent equivalent to the coadsorption capacity of the desiccant bed is then added to the original CO_2-sorbent, and the program rerun for NCT2 cycles to obtain the performance of the bed at NCT1 cycles from the beginning, accounting for the coadsorption effect.

In the present example, the Airlock RCRS performance is simulated at 2-days into a mission. The accumulation of H_2O is established by running the program for 96 cycles (half-cycle being 15 minutes), deliberately using an over-sized desiccant section. Pertinent data required for the run are given in Figure 9-4. A total of 18 nodes are used, nine being CO_2 sorbents. The split of sorbents for CO_2 and H_2O is given in Figure 9-5. The program is run for 96 complete cycles (NCT1=96), the coadsorption capacity of the desiccant for CO_2 is calculated at the water loadings prevailing and sorbent bed sizes adjusted accordingly. The new bed sizes are shown in Figure 9-6. The performance of the new bed is then obtained by running the program for 14 complete cycles (NCT2=14). Print-outs at the adsorption and desorption end of the 14th cycle are shown in Figures 9-7 and 9-8. The adsorption half-cycle performance computed by the program is compared with test data (Reference 8) in Figure 9-9. The output P_{CO_2}'s as predicted by the program matches the test results reasonably well; the inlet P_{CO_2}'s as shown are quite different; however, a material balance of the system indicates that the test data are in error, possibly caused by instrumentation line leakage. Figure 9-10 compares the desorption pressures computed by the program with test data. The match is good.

```
$MAIN
AM       =    .44000000+02,    .18000000+02,
CYCLE    =    .25000000+00,
DTMAX    =    .49999999-02,
WI       =    .49999999-02,
TI       =    .25000000+01,
PCO2C    =    .55000000+01,
VOLCAB   =    .70000000+02,
RCO2C    =    .28100000+00,
NPRINT   =              30,
NDICON   =               1,
NTEMP    =               1,
TGC      =    .65000000+02,
PAC      =    .25900000+03,
PH2OC    =    .10000000+02,
TGHX     =    .20000000+03,
PCO2A    =    .25000000+02,
VCO2A    =    .10000000+02,
SABCO2   =    .79499999+00,
TCO2A    =    .10000000+03,
KBED     =               ,                1,                ,                ,
TIMEDS   =    .20000000+01,
NCT1     =              96,
NST1     =              96,
NCT2     =              14,
NST2     =              14,
$END
$B1M
PA1      =    .00000000+00,
TSU1     =    .35000000+03,    .35000000+03,    .35000000+03,    .35000000+03,
              .35000000+03,    .35000000+03,    .35000000+03,    .35000000+03,
              .35000000+03,    .35000000+03,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TCU1     =    .35000000+03,    .35000000+03,    .35000000+03,    .35000000+03,
              .35000000+03,    .35000000+03,    .35000000+03,    .35000000+03,
              .35000000+03,    .35000000+03,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
TX01     =    .35000000+03,    .35000000+03,    .35000000+03,    .35000000+03,
              .35000000+03,    .35000000+03,    .35000000+03,    .35000000+03,
              .35000000+03,    .35000000+03,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
              .00000000+00,    .00000000+00,    .00000000+00,    .00000000+00,
W1       =    .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
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              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
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              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
              .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
```

Figure 9-4. Input Data for Example No. 2

```
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
                .10000000-02,    .10000000-02,    .10000000-02,    .10000000-02,
GMR1     =      .67000000+02,
GMW1     =      .29500000+02,
PN21     =      .00000000+00,
PO21     =      .00000000+00,
$END
$B2M
PA2      =      .25800000+03,
TS02     =      .68000000+02,    .68000000+02,    .68000000+02,    .68000000+02,
                .68000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .70000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .60000000+02,    .50000000+02,    .40000000+02,    .35000000+02,
                .30000000+02,    .20000000+02,    .00000000+00,    .00000000+00,
TC02     =      .70000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .70000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .70000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .70000000+02,    .70000000+02,    .65000000+02,    .65000000+02,
                .65000000+02,    .70000000+02,    .00000000+00,    .00000000+00,
TX02     =      .68000000+02,    .68000000+02,    .68000000+02,    .68000000+02,
                .68000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .70000000+02,    .70000000+02,    .70000000+02,    .70000000+02,
                .60000000+02,    .50000000+02,    .40000000+02,    .35000000+02,
                .30000000+02,    .20000000+02,    .00000000+00,    .00000000+00,
W2       =      .23500000-01,    .23500000-01,    .23500000-01,    .23500000-01,
                .24100000-01,    .24100000-01,    .24100000-01,    .24100000-01,
                .23800000-01,    .23800000-01,    .23800000-01,    .23800000-01,
                .23300000-01,    .23300000-01,    .23300000-01,    .23300000-01,
                .22800000-01,    .22800000-01,    .22800000-01,    .22800000-01,
                .22100000-01,    .22100000-01,    .22100000-01,    .22100000-01,
                .29300000-01,    .29300000-01,    .29300000-01,    .29300000-01,
                .29800000-01,    .29800000-01,    .29800000-01,    .29800000-01,
                .30300000-01,    .30300000-01,    .30300000-01,    .30300000-01,
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                .49999999-01,    .49999999-01,    .49999999-01,    .49999999-01,
                .49999999-01,    .49999999-01,    .49999999-01,    .49999999-01,
                .69999998-01,    .69999998-01,    .69999998-01,    .69999998-01,
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GMR2     =      .15500000+02,
GMW2     =      .31000000+02,
PN22     =      .65000000+02,
PO22     =      .19300000+03,
$END
$B3M
PA3      =      .00000000+00,
TS03     =      .45000000+02,    .45000000+02,    .45000000+02,    .45000000+02,
                .45000000+02,    .45000000+02,    .45000000+02,    .45000000+02,
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                .45000000+02,    .45000000+02,    .45000000+02,    .45000000+02,
TC03     =      .45000000+02,    .45000000+02,    .45000000+02,    .45000000+02,
                .45000000+02,    .45000000+02,    .45000000+02,    .45000000+02,
```

Figure 9-4. (Continued)

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                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
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HXC      =       .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
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                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
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                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
HSG      =       .20000000+02,      .20000000+02,      .20000000+02,      .20000000+02,
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                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
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SK       =       .00000000+00,      .99999998-01,      .99999998-01,      .99999998-01,
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TKX      =       .00000000+00,      .90000000+01,      .90000000+01,      .90000000+01,
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DH       =       .14000000+04,      .14000000+04,      .14000000+04,      .14000000+04,
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                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
DIF      =       .40000000-04,      .40000000-04,      .40000000-04,      .40000000-04,
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GK       =       .49999999-02,      .49999999-02,      .49999999-02,      .49999999-02,
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TCIN     =       .00000000+00,
HTR1     =       .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
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                 .00000000+00,      .00000000+00,      .00000000+00,      .00000000+00,
TMAX     =       .40000000+03,
WCC      =       .00000000+00,
$END
$MB
ABED     =       .42600000+00,      .42600000+00,      .42600000+00,      .38000000+00,
                 .38000000+00,      .38000000+00,      .38000000+00,      .38000000+00,
                 .38000000+00,      .42600000+00,      .42600000+00,      .42600000+00,
                 .42600000+00,      .42600000+00,      .42600000+00,      .42600000+00,
                 .42600000+00,      .42600000+00,      .00000000+00,      .00000000+00,
AVC      =       .10000000+03,      .10000000+03,      .10000000+03,      .10000000+03,
                 .10000000+03,      .10000000+03,      .10000000+03,      .10000000+03,
                 .10000000+03,      .10000000+03,      .10000000+03,      .10000000+03,
                 .10000000+03,      .10000000+03,      .10000000+03,      .10000000+03,
                 .10000000+03,      .10000000+03,      .00000000+00,      .00000000+00,
ASX      =       .61799999+01,      .61799999+01,      .61799999+01,      .61799999+01,
```

Figure 9-4. (Continued)

		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.00000000+00,	.00000000+00,
AGX	=	.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.61799999+01,	.61799999+01,
		.61799999+01,	.61799999+01,	.00000000+00,	.00000000+00,
AVX	=	.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.37500000+03,	.37500000+03,
		.37500000+03,	.37500000+03,	.00000000+00,	.00000000+00,
RHOG	=	.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
		.30000000-03,	.30000000-03,	.30000000-03,	.30000000-03,
RHOSB	=	.43000000+02,	.43000000+02,	.43000000+02,	.36000000+02,
		.36000000+02,	.36000000+02,	.36000000+02,	.36000000+02,
		.36000000+02,	.43000000+02,	.43000000+02,	.43000000+02,
		.43000000+02,	.43000000+02,	.43000000+02,	.43000000+02,
		.43000000+02,	.43000000+02,	.00000000+00,	.00000000+00,
RHOS	=	.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.64000000+02,	.64000000+02,
		.64000000+02,	.64000000+02,	.00000000+00,	.00000000+00,
RHOC	=	.11500000+03,	.11500000+03,	.11500000+03,	.11500000+03,
		.11500000+03,	.11500000+03,	.11500000+03,	.11500000+03,
		.11500000+03,	.11500000+03,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
RHOX	=	.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.49000000+03,	.49000000+03,
		.49000000+03,	.49000000+03,	.00000000+00,	.00000000+00,
CPG	=	.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.23000000+00,	.23000000+00,
		.23000000+00,	.23000000+00,	.00000000+00,	.00000000+00,
CPC	=	.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.10000000+21,	.10000000+21,
		.10000000+21,	.10000000+21,	.00000000+00,	.00000000+00,
CPX	=	.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.10999999+00,	.10999999+00,
		.10999999+00,	.10999999+00,	.00000000+00,	.00000000+00,
CPP	=	.25000000+00,	.25000000+00,	.25000000+00,	.35100000+00,
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		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
		.25000000+00,	.25000000+00,	.25000000+00,	.25000000+00,
DX	=	.55599999-01,			

Figure 9-4. (Continued)

```
NPSET   =                 ,                ,               10,
NDR4    =                2,
NDXMAC  =                9,
NBCOUT  =                1,
NDX1    =               18,
NDXM    =                9,
NOG     =                1,
POUT    =   .11000000+02,   .33000000+01,   .24500000+03,   .57500000+03,
            .33700000+03,   .11700000+03,   .82000000+02,   .52000000+02,
            .45000000+02,   .34400000+02,
TIMET   =   .10000000-04,   .20000000-02,   .89999998-01,   .19000000+00,
            .30000000+00,   .59999999+00,   .75000000+00,   .10500000+01,
            .12000000+01,   .20000000+01,
PUMP    =   .00000000+00,   .45000000+00,   .50000000+00,   .90000000+01,
            .10000000+04,   .25000000+02,   .25000000+02,   .25000000+02,
            .25000000+02,   .25000000+02,
VPUMP   =   .25000000+05,   .25000000+05,   .13000000+05,   .13000000+05,
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            .00000000+00,   .00000000+00,
IDSORB  =              1,              1,              1,              1,
                       1,              1,              1,              1,
                       1,              1,              1,              1,
                       3,              3,              3,              3,
                       3,              3,              3,              3,
CPL     =   .10200000+01,   .10000000+01,
DP      =   .64199999-02,   .64199999-02,   .64199999-02,   .64199999-02,
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$END
$MBA
HXG     =   .10099999+00,   .10099999+00,   .10099999+00,   .10099999+00,
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HXS     =   .68499999+00,   .68499999+00,   .68499999+00,   .79500000+02,
            .79500000+02,   .79500000+02,   .79500000+02,   .79500000+02,
            .79500000+02,   .68499999+00,   .68499999+00,   .68499999+00,
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            .68499999+00,   .20000000+01,   .00000000+00,   .00000000+00,
HXC     =   .20000000+00,   .20000000+00,   .20000000+00,   .20000000+00,
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HSG     =   .20000000+02,   .20000000+02,   .20000000+02,   .20000000+02,
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SK      =   .00000000+00,   .99999998-01,   .99999998-01,   .58000000+01,
            .11600000+02,   .11600000+02,   .11600000+02,   .11600000+02,
            .11600000+02,   .58000000+01,   .99999998-01,   .99999998-01,
            .99999998-01,   .99999998-01,   .99999998-01,   .99999998-01,
            .99999998-01,   .99999998-01,   .00000000+00,   .00000000+00,
TKX     =   .00000000+00,   .90000000+01,   .90000000+01,   .90000000+01,
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            .90000000+01,   .90000000+01,   .90000000+01,   .90000000+01,
```

Figure 9-4. (Continued)

```
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                  .90000000+01,   .90000000+01,   .00000000+00,   .00000000+00,
DH        =       .40000000+03,   .40000000+03,   .40000000+03,   .40000000+03,
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DIF       =       .99999998-04,   .99999998-04,   .99999998-04,   .99999998-04,
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GK        =       .49999999-03,   .49999999-03,   .49999999-03,   .49999999-03,
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TCIN      =       .00000000+00,
HTR1      =       .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
                  .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
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                  .00000000+00,   .00000000+00,   .00000000+00,   .00000000+00,
TMAX      =       .40000000+03,
WCC       =       .00000000+00,
$END
$MBD
HXG       =       .15100000-01,   .15100000-01,   .15100000-01,   .15100000-01,
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HXS       =       .55000000+00,   .55000000+00,   .55000000+00,   .79500000+02,
                  .79500000+02,   .79500000+02,   .79500000+02,   .79500000+02,
                  .79500000+02,   .55000000+00,   .55000000+00,   .55000000+00,
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                  .55000000+00,   .18000000+01,   .00000000+00,   .00000000+00,
HXC       =       .20000000+00,   .20000000+00,   .20000000+00,   .20000000+00,
                  .20000000+00,   .20000000+00,   .20000000+00,   .20000000+00,
                  .20000000+00,   .20000000+00,   .20000000+00,   .20000000+00,
                  .20000000+00,   .69999999+00,   .33000000+01,   .33000000+01,
                  .33000000+01,   .33000000+01,   .00000000+00,   .00000000+00,
HSG       =       .30000000+01,   .30000000+01,   .30000000+01,   .30000000+01,
                  .30000000+01,   .30000000+01,   .30000000+01,   .30000000+01,
                  .30000000+01,   .30000000+01,   .30000000+01,   .30000000+01,
                  .30000000+01,   .30000000+01,   .30000000+01,   .30000000+01,
                  .30000000+01,   .30000000+01,   .00000000+00,   .00000000+00,
SK        =       .00000000+00,   .79999998-01,   .79999998-01,   .58000000+01,
                  .11600000+02,   .11600000+02,   .11600000+02,   .11600000+02,
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TKX       =       .00000000+00,   .90000000+01,   .90000000+01,   .90000000+01,
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                  .90000000+01,   .90000000+01,   .90000000+01,   .90000000+01,
                  .90000000+01,   .90000000+01,   .00000000+00,   .00000000+00,
DH        =       .40000000+03,   .40000000+03,   .40000000+03,   .40000000+03,
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```

Figure 9-4. (Continued)

```
                 .14000000+04,     .14000000+04,     .14000000+04,     .14000000+04,
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DTF      =       .99999998-04,     .99999998-04,     .99999998-04,     .99999998-04,
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                 .99999998-04,     .99999998-04,     .99999998-04,     .99999998-04,
GK       =       .49999999-03,     .49999999-03,     .49999999-03,     .49999999-03,
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                 .10000000-02,     .10000000-02,     .10000000-02,     .10000000-02,
                 .10000000-02,     .10000000-02,     .10000000-02,     .10000000-02,
TCIN     =       .00000000+00,
HTR1     =       .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                 .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                 .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                 .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
                 .00000000+00,     .00000000+00,     .00000000+00,     .00000000+00,
TMAX     =       .40000000+03,
WCC      =       .00000000+00,
$END
```

Figure 9-4. (Continued)

BED NO 2

VOLUME AND WEIGHT

BULK VOLUME OF CO2 SORBENT (CU FT)	.1978
WEIGHT OF CO2 SORBENT (LB)	7.6191
WEIGHT OF ACTIVE CO2 SORBENT (LB)	7.6191
BULK VOLUME OF DESICCANT (CU FT)	.2132
WEIGHT OF DESICCANT (LB)	9.1663

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0291
OXYGEN LOSS (LB/HR)	.0338

Figure 9-5. Initial Sorbent Bed Size for Example No. 2

BED NO 2

VOLUME AND WEIGHT

BULK VOLUME OF CO2 SORBENT (CU FT)	.2452
WEIGHT OF CO2 SORBENT (LB)	9.2227
WEIGHT OF ACTIVE CO2 SORBENT (LB)	9.2227
BULK VOLUME OF DESICCANT (CU FT)	.1658
WEIGHT OF DESICCANT (LB)	7.5627

ESTIMATED CABIN GAS LOSSES

NITROGEN LOSS (LB/HR)	.0348
OXYGEN LOSS (LB/HR)	.0395

Figure 9-6. Sorbent Bed Sizes After 2 Days, Accounting for Coadsorption

BED NO. 2

ADSORPTION CYCLE 14
TIME= .25000 HR 15.000 MIN TIME INCREMENT= .00116 HR

AXIAL NODE	PCO2,MM	PH2O,MM	GAS TEMP, F	SORBENT TEMP, F	COOLANT TEMP, F	HX CORE TEMP, F
1	2.4117	.0380	71.5703	71.5572	69.9997	70.5092
2	2.6671	.0380	72.6753	72.6678	69.9997	70.9539
3	2.9419	.0380	73.3119	73.3130	69.9997	71.7848
4	3.2348	.0380	73.2267	73.2275	69.9997	73.0470
5	3.4793	.0380	73.1696	73.1708	69.9997	73.1090
6	3.7368	.0380	73.0848	73.0867	69.9997	73.0426
7	4.0124	.0380	72.9480	72.9509	69.9997	72.9147
8	4.2923	.0380	72.7445	72.7484	69.9997	72.7151
9	4.5699	.0380	72.4694	72.4742	69.9997	72.4149
10	4.8392	.0380	72.1309	72.1372	69.9997	71.7272
11	5.1832	.0380	71.6630	71.6666	69.9997	71.1444
12	5.3367	.0380	71.5102	71.4400	69.9997	70.7924
13	5.3367	.2626	77.0589	76.8581	69.9997	70.9627
14	5.3367	1.1042	92.9287	92.7268	69.9997	71.5828
15	5.3367	3.9261	108.9492	108.9993	64.9997	71.5795
16	5.3367	7.0879	105.1354	105.2829	64.9997	71.5911
17	5.3367	8.5228	92.2183	92.3694	64.9997	71.5058
18	5.3367	9.3505	78.9322	79.0899	69.9997	72.3010
INLET	5.3367	10.0000	65.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB

AXIAL NODE \ SORB NODE	AVG	1	2	3	4
1	.0334	.0331	.0336		
2	.0346	.0343	.0349		
3	.0361	.0358	.0364		
4	.0381	.0378	.0385		
5	.0398	.0394	.0402		
6	.0416	.0412	.0420		
7	.0435	.0431	.0440		
8	.0456	.0452	.0460		
9	.0477	.0473	.0481		
10	.0498	.0494	.0502		
11	.0525	.0522	.0528		
12	.0929	.0928	.0929		
13	.1505	.1502	.1508		
14	.1744	.1734	.1755		
15	.1969	.1954	.1984		
16	.2136	.2129	.2144		
17	.2272	.2268	.2276		
18	.2388	.2385	.2391		

AVG CO2 LOADING IN CO2 SORBENT (LB/LB) @@@@@@@@@@@@ .0415 AVG H2O LOADING IN DESICCANT (LB/LB) @@@@@@@@@@@@ .1849
TIME AVG CO2 ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ .2609 TIME AVG H2O ADSORPTION RATE (LB/HR) @@@@@@@@@@@@ .3480

ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)@@@@@@ .0000 HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)@@@@@@ -.0000
TIME AVG OUTLET PH2O (MM) @@@@@@@@@@@@@@@@@@@@@@@@ .0233

Figure 9-7. Print-Out at End of Adsorption Half-Cycle

BED NO. 2

DESORPTION CYCLE 14
TIME= .25000 HR 15.000 MIN TIME INCREMENT= .00368 HR

AXIAL NODE	TOTAL PRESS,MM	GAS TEMP,DEG F	SORBENT TEMP, DEG F	COOLANT TEMP,DEG F	HX CORE TEMP, DEG F
1	1.7384	68.1609	68.1609	69.9997	68.7299
2	1.7280	67.7145	67.7144	69.9997	68.2075
3	1.7074	66.8417	66.8415	69.9997	67.1297
4	1.6788	65.3593	65.3586	69.9997	65.4254
5	1.6464	63.7844	63.7834	69.9997	63.8385
6	1.6076	62.1667	62.1655	69.9997	62.2232
7	1.5621	60.5090	60.5076	69.9997	60.5712
8	1.5098	58.8138	58.8122	69.9997	58.9089
9	1.4503	57.0826	57.0807	69.9997	57.5427
10	1.3779	55.2748	55.2728	69.9997	60.1886
11	1.3153	53.5110	53.5068	69.9997	62.3856
12	1.2457	71.0161	71.0373	69.9997	64.5047
13	1.1134	71.1168	71.1171	69.9997	65.5250
14	.9735	70.3106	70.3099	69.9997	65.5660
15	.8175	63.6929	63.6850	64.9997	64.4506
16	.6388	52.7621	52.7474	64.9997	62.8547
17	.4322	38.8388	38.8178	64.9997	60.8153
18	.1814	25.2948	25.2683	69.9997	58.3382

LOADING AT INTERIOR OF SORBENT

AXIAL NODE \ SORB NODE	AVG	1	2	3	4
1	.0313	.0316	.0310		
2	.0315	.0318	.0312		
3	.0319	.0322	.0316		
4	.0327	.0330	.0324		
5	.0334	.0337	.0331		
6	.0342	.0345	.0339		
7	.0349	.0352	.0346		
8	.0355	.0358	.0352		
9	.0361	.0364	.0357		
10	.0366	.0369	.0362		
11	.0368	.0372	.0365		
12	.0927	.0927	.0927		
13	.1488	.1489	.1487		
14	.1689	.1691	.1687		
15	.1839	.1842	.1837		
16	.1961	.1964	.1958		
17	.2080	.2083	.2077		
18	.2164	.2168	.2160		

AVG CO2 LOADING IN CO2 SORBENT (LB/LB) @@@@@@@@@@@@ .0339
TIME AVG CO2 DESORPTION RATE (LB/HR) @@@@@@@@@@@@ .2797
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)@@@@@@ .0000

AVG H2O LOADING IN DESICCANT (LB/LB) @@@@@@@@@@@@ .1735
TIME AVG H2O DESORPTION RATE (LB/HR) @@@@@@@@@@@@ .3440
HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)@@@@@@ -.0000

ACCUMULATOR CO2 PRESSURE (PSIA) @@@@@@@@@@@@@@@@@@ 25.0000

CO2 ACCUMULATOR VOLUME (CU FT) @@@@@@@@@@@@@@@@@@ 10.0000

Figure 9-8. Print-Out at End of Desorption Half-Cycle

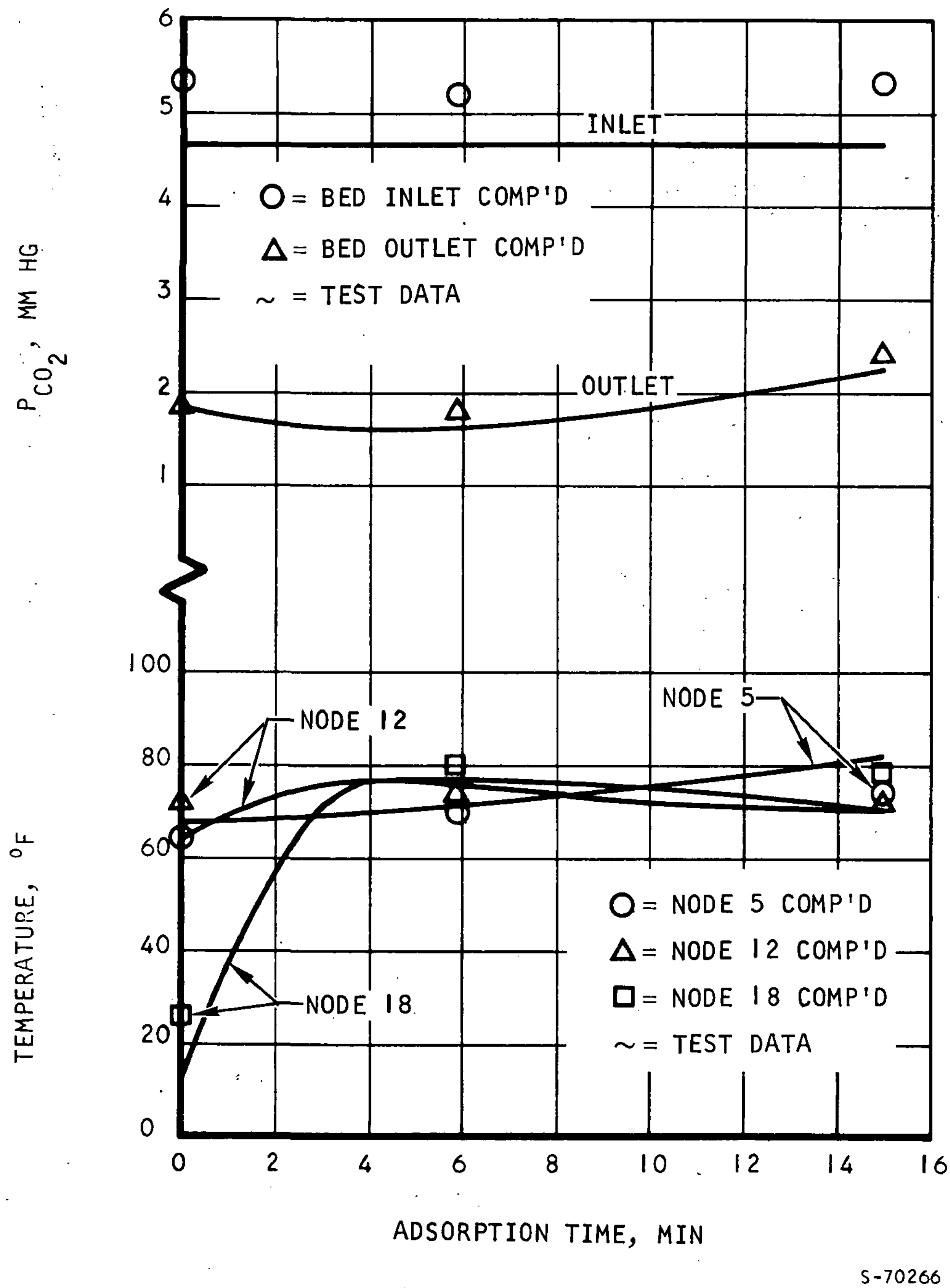

Figure 9-9. Comparison of Computed Adsorption Cycle Performance with Test Data (Cycle 94 of 28 Day Test); Lines

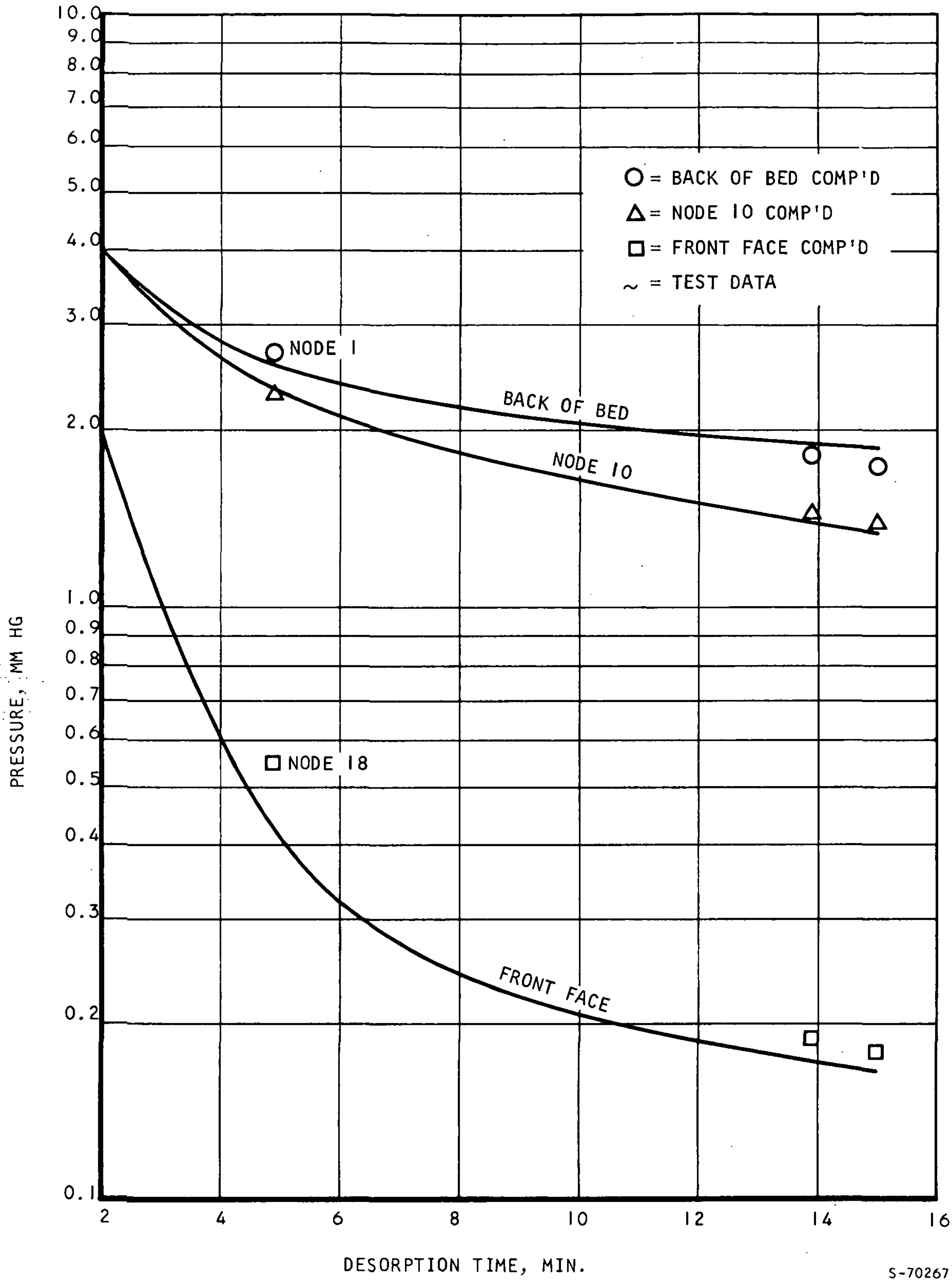

Figure 9-10. Comparison of Computed Desorption Pressures with Test Data (Cycle 94 of 28 Day Test)

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APPENDIX A

SUBPROGRAM DOCUMENTATION

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APPENDIX A

SUBPROGRAM DOCUMENTATION

This appendix contains descriptions of newly developed subprograms for program MAIN4B. The reader is referred to the original single bed program S9960 (Part I of this report) for the description of the old subprograms.

ADSØRB

Adsorption/gas stripping subroutine. Refer to Part I of this report.

BED4

The creation of this subroutine was necessitated by the impracticability of transferring all the bed data required in various subroutines, from one subroutine to another. There are a maximum of four beds in the system, and these data must be stored in different locations. A primary function of BED4 is to transfer the bed data stored under dummy bed variables RDB, IDB, RMB, etc., to the actual variables used in adsorption/desorption subroutines, such as TG, ABED, etc., and vice versa. A logic diagram of BED4 is given in Figure A-1. It is apparent that, in addition to storage transfers, the subroutine controls various options and printouts.

DESØRB

This subroutine performs vacuum desorption calculations and is an expanded version of the original subroutine S9983.

The new version uses a more generally applicable analysis of the vacuum duct, and for a CO_2-save system, vacuum pump characteristics can be inputted.

EQPWT

This is a new equilibrium data subroutine, which uses a two dimensional interpolation scheme to find the equilibrium pressure or loading corresponding respectively to a given set of loading and temperature or pressure and temperature. Arguments of the subroutine are:

ID = Index identifying sorbate, 1 for CO_2, 2 for H_2O, 3 for N_2, 4 for O_2.

IDSØRB = Index identifying sorbent, 1 for 5A, 2 for S.G., 3 for 13X, 4 for 4A, 5 for 3A.

KPW = Control index, 1 to find P, given W and T, 2 to find W, given P and T.

P = Vapor pressure of sorbate, mm Hg.

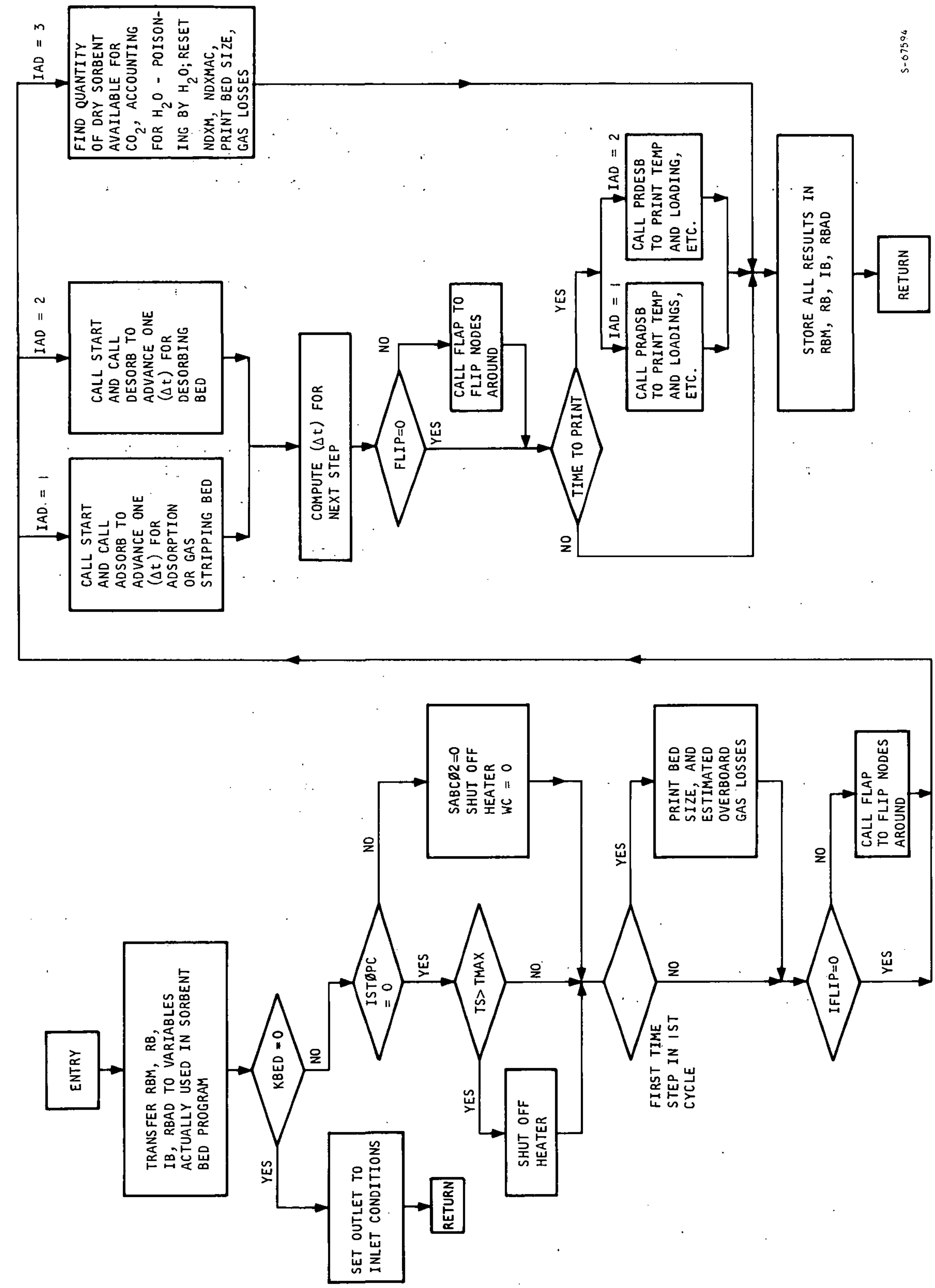

Figure A-1. Logic Diagram for Subroutine BED4

W = Loading, (lb sorbate)/(lb dry sorbent)

T = Temperature, ^{o}F

The equilibrium data currently available for various sorbate-sorbent systems are stored in the subroutine in the form of data statements. The variable names used for these data are:

TTAB (NT(IS),IS) = Temperature, ^{o}F

WTAB (K,NT(IS),IS) = Loading, (lb sorbate)/(lb dry sorbent)

PTAB (K,NT(IS),IS) = vapor pressure, mm Hg

NT (IS) = Number of temperatures at which W versus P are tabulated for IS system

IDSMTX (IDSØRB,ID) = A two-dimensional array which tabulates IS for each combination of IDSØRB and ID; refer to Table A-1.

FCØAD

This function subprogram determines fractional effectiveness of partially water-poisoned sorbents for CO_2 adsorption by table look-ups.

The coadsorption data are stored as FCØADT (I, IDSØRB) versus H2ØT(I), I = 1 to 12.

FDEQID

No changes made; refer to Part I of this report.

FDEQIM

Same; refer to Part I of this report.

FLAP

This subroutine switches bed properties around; node 1 interchanges with node NDX1, node 2 interchanges with node (NDX1-1), and so forth. This is required when the gas flow direction is reversed as is the case where gas stripping is used to regenerate a bed.

FLIP

A subroutine used by FLAP.

FLØP

A subroutine used by FLAP.

TABLE A-1

TABULATION OF IS FOR EACH
COMBINATION OF IDSORB AND ID

IDSORB \ ID / IS	1 (CO_2)	2 (H_2O)	3 (N_2)	4 (O_2)	5
1 (5A)	1	2	6	7	
2 (S.G.)		3			
3 (13X)	4	5	8	9	
4 (4A)					
5 (3A)					

GAST

Refer to Part I of this report.

GASTA

Refer to Part I of this report.

HXCØRE

Same as HXCØRE in the original program except that it now solves Equation (4), which has a source term to account for the heater output.

IFN

Refer to Part I of this report.

LAGIN2

Refer to Part I of this report.

NEWTØ2

An iteration routine using the Newton-Wegstein method.

Arguments of the subroutine are:

NI = Control index indicating the total number of iterations made; NI should be set equal to 1 before NEWTØ2 is called.

NGØ = Output index; 1 for conversion still unreached, 2 for conversion reached

X = Independent variable; value of X to be found such that Y = 0.

Y = Dependent variable, which should approach zero as a conversion is attained.

X0 = Previous value of X.

Y0 = Previous value of Y.

XMIN = Minimum limit for X.

XMAX = Maximum limit for X.

ER = Conversion criterion. If $|Y| < ER$ conversion has been reached.

PRADSB

Refer to Part I of this report.

PRDESB

Refer to Part I of this report.

PRDESB

Refer to Part I of this report.

READ1

The subroutine reads in namelists 'DB' and 'DBA'.

READ2

The subroutine reads in namelist 'DBD'.

READ3

The subroutine reads in namelists 'MB' and 'MBA'.

READ4

The subroutine reads in namelist 'MBD'.

START

This is a subroutine to replace the original START and STARTA.

TGLCØL

Refer Part I of this report.

TSØRB

Refer to Part I of this report.

TSØRBA

Refer to Part I of this report.

XYZMAP

This is a two-dimensional interpolation routine. The argument variables are:

IND = Option index: IND = 0, Z = F(X,Y); IND = 1, Y = F(X,Z); IND = -1, Y = F(X).

X,Y,Z = Independent and dependent variables.

NP = Number of points per curve, or number of X,Y pairs for each Z.

NC = Number of curves, i.e., number of Z-values.

IDX = Number of data points to be used in interpolating in X - direction.

IDY = Number of data points to be used in interpolating in Y - direction.

BX = First independent variable.

BY = Second independent variable.

ANS = Dependent variable found corresponding to BX, BY. In another word, = XYZMAP.

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APPENDIX B

PROGRAM LISTING

APPENDIX B

PROGRAM LISTING

This appendix contains a total listing of program MAIN4B.

```
@ ELT ADSORB,1,710719, 62333   , 1
                SUBROUTINE ADSORB
                COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,       PK (2,20),PCO2I  ,TS  (20)     *NEW
               1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),       *NEW
               2TC2 (20),W (4,20),PT (20),         GMR ,GMW,GVIS, PN2,PO2,              *NEW
               3           ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),            *NEW
               4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                 *NEW
               5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                      *NEW
               6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),            *NEW
               7NPSET(5),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                  *NEW
               8                                 HXG(20),HXS(20),HXC(20),HSG(20),      *NEW
               9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,       *NEW
               1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                     *NEW
               1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,              *NEW
               1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),      *NEW
               1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),       *NEW
               2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),        *NEW
               3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3    *NEW
               4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),     *NEW
               5              WM(2),TIME,CYCLE,DTO,    DTMAX,WI,TI,PCO2C,              *NEW
               6VOLCAB,RCO2C,                                                          *NEW
               7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS          *NEW
                DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,              *NEW
               1      CP1,CP2,X,    C1P,C2P,C3P,D1P                                     *NEW
                DIMENSION AS(20)                                                       **-1
                EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
               1,HGS)
                DATA RGAS/554./
          C
                NDR=NDR4-1
                DO 21 N=1,NDX1
                AS(N)=4.*3.1416*RS(N)**2
                I=N
                DO 20 NR=1,NDR4
                C1(NR,N)=-CR2(I,NR)
                C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
             20 C3(NR,N)=-CR3(I,NR)
          C
          C
                B(1,N)=C3(1,N)/C2(1,N)
                DO 21 J=2,NDR
             21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
                NDX=NDX1-1
          C     TO TEMPORARILY STORE SURFACE LOADING
                DO 50 N=1,NDX1
           50   WS(N)=W(NDR4,N)
                IF (NTEMP .EQ. 0 ) GO TO 111
          C
          C     TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
                DO 12 N=1,NDX1
                I=IFN(N,NDXM)
                CS2(N)=DT/CPS(N)/RHOSB(N)*ASG(N)*GK(N)*WM(I)*DH(N)
                CS1(N) = CS2(N)
                IF (N.EQ.1) GO TO 13
                IF (N.EQ.NDX1) GO TO 14
                S1=SK(N)/DX**2*(TS(N-1)-2.*TS(N)+TS(N+1))
                GO TO 15
             13 S1=SK(1)/DX**2*(TS(2)-TS(1))
                GO TO 15
```

```
   14 S1=SK(NDX1)/DX**2*(TS(NDX)-TS(NDX1))
   15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+
     1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
      RATIO = (DT+DTO)/DT
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=RATIO*CS1(N)/(1.+T1)
      CS2(N)=RATIO*CS2(N)/(1.+T1)
      DS(N)=RATIO*DS(N)
      DS(N)= (DS(N)-T1*TS2(N))/(1.+T1)
   12 CONTINUE
      GO TO 110
  111 DO 112 N= 1, NDX1
      CS1(N)=0.
      CS2(N)=0.
      DS(N)=0.
      TS(N)=T268
      TC(N)=T268
      TX(N)=T268
      TG(N)=T268
  112 CONTINUE
  110 CONTINUE
C
C     TO CALCULATE PARTIAL PRESSURE OF ADSORBATE IN GAS STREAM
C
      DO 24 N=1,NDX1
      I=IFN(N,NDXM)
C     TO CALCULATE P1,P2,P3
      WSURF=W(NDR4,N)
      CALL EQPWT(I,IDSORB(N),1,PSURF,WSURF,TS2(N))
      CALL EQPWT(I,IDSORB(N),1,PS1,    WSURF,(TS2(N)+0.02))
      DPKDTS=(PS1-PSURF)/0.02
      CALL EQPWT(I,IDSORB(N),1,PS2,(WSURF+1.E-5),TS2(N))
      DPKDWK=(PS2-PSURF)/1.E-5
      G=1.+CS2(N)*DPKDTS
      P1(N)=(PSURF                    +DS(N)*DPKDTS)/G
      P2(N)=DPKDWK/G
      P3(N)=CS1(N)/G*DPKDTS
C
      C2(NDR4,N)=CR1(N,NDR4)/DT+CR2(N,NDR4)+WM(I)*GK(N)*P2(N)*AS(N)
      C3(NDR4,N)=0.0
      DO 23 NR=1,NDR4
   23 D1(NR,N)=CR1(N,NR)/DT*W(NR,N)
      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(N)
      D2(N)=AS(N)*WM(I)*GK(N)*( 1.     -P3(N))
      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))
      Q(1,N)=D1(1,N)/C2(1,N)
      DO 24 J=2,NDR4
   24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
C
      DO 25 N=1,NDX1
      I=IFN(N,NDXM)
      CP1(N)=ASG(N)*GK(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
   25 CP2(N)=ASG(N)*GK(N)*(P2(N)*D2(N)+P3(N)-1.0)
      PK(1,NDX1+1) = PCO2I
      PK(2,NDX1+1) = PH2OI
      DO 26 N=1,NDX1
      N1=NDX1+1-N
      I=IFN(N1,NDXM)
      PK(I,N1) = (PK(I,N1+1)/DX+CP1(N1)/A(N1))
```

```
                 1                                   /(1./DX-CP2(N1)/A(N1))
                  IF (I.EQ.1)J=2
                  IF(I.EQ.2)J=1
                  PK(J,N1)=PK(J,N1+1)
               26 CONTINUE
            C
            C
            C
            C     TO CALCULATE SORBENT LOADING
            C
                  DO 30 N=1,NDX1
                  I=IFN(N,NDXM)
                  W(NDR4,N)=Q(NDR4,N)+D2(N)*PK(I,N)
                  DO 30 J=2,NDR4
                  L=NDR4+1-J
               30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
            C
            C
                  IF( NTEMP .EQ. 0) RETURN
            C     TO CALCULATE SORBENT,GLYCOL,HX CORE AND GAS TEMPERATURES
            C
                  CALL TSORBA
                  CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
                 1AVC, NOG    ,DTO,TS1,TS2,TX1,TX2,TC1,TC2)
                  CALL HXCORE
                  CALL GASTA(GMR,CPG,ABED,NDX1,TGI,ASG,HSG,AXG,HXG,DX,TG,TS,TX)
                  RETURN
                  END
```

```
@ ELT BED4,1,710720, 31270      , 1
      SUBROUTINE BED4(IBED,IFLIP,IAD,RBM,RB,IB,RBAD,ISTOPC,KBED)
      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,       PK (2,20),PCO2I  ,TS  (20)
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
     2TC2 (20),W (4,20),PT (20),           GMR ,GMW,GVIS, PN2,PO2,
     3                ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
     4AVX(20),RHOG(20),RHOS3(20),RHOS(20),RHOC(20),RHOX(20),
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
     8                                 HXG(20),HXS(20),HXC(20),HSG(20),
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,
     1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
     3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
     5                WM(2),TIME,CYCLE,DTO,   DTMAX,WI,TI,PCO2C,
     6VOLCAB,RCO2C,
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
     1        CP1,CP2,X,   C1P,C2P,C3P,D1P
      DIMENSION RBM(1), RB(1), IB(1), RBAD(1),KBED(1)
      DIMENSION WN(20)
C  IFLIP =0, NO FLIP,   IFLIP=1,  FLIP WILL BE CALLED
      DATA ISTART/0/
C
      DO 110 N=1,349
  110 TG(N)=RBM(N)
      DO111 N=1, 405
  111 ABED(N)=RB(N)
      DO112 N= 1,29
  112 NPSET(N)=IB(N)
      DO 13 N=1,251
   13 HXG(N)=RBAD(N)
      IF(KBED(IBED) .EQ. 0)   GO TO 90
 8976 FORMAT(I25)
      NDX10=NDX1                        @ THESE TWO CARDS ARE ENTROPY GENERATORS
      NDX1=NDX10
      SABCO2=SABCOS
      IF(ISTOPC .NE. 0) SABCO2=0.0
      DO 1311 N= 1, NDX1
      HTR(N)=HTR1(N)
      IF(ISTOPC .NE. 0) GO TO 3198
      IF(TS(N) .GT. TMAX) GO TO 3198
      GO TO 1311
 3198 DO 411 J= 1, NDX1
  411 HTR(J) = 0.0
      GO TO 66
 1311 CONTINUE
   66 CONTINUE
      ISTART=ISTART+1
      IF(TIME .LT. 1.1E-5) GO TO 80
      GO TO 81
   80 SUMPTM=0.0
      TOTKWH=0.0
      TOTCO2=0.0
```

```
      TOTH2O=0.
      TOTHTC=0.0
      IF(ISTART .GT. 4) GO TO 81
C
      ASSIGN 82 TO NPRSBR
      GO TO 183
   82 CONTINUE
C
   81 WC=WCC
      IF(ISTOPC.NE.0) WC=0.
      DO 801 N=1,NDX1
      AC=ABED(N)*ASX(N)/AVC(N)
  801 UC(N)=WC/AC/RHOC(N)
      IF(IFLIP.NE.0) CALL FLAP
   15 GO TO (16,17,18     ), IAD
   16 CALL START
      CALL ADSORB
      SUMPTM= SUMPTM+PK(2,1)*DT
      GO TO 19
   17 CALL START
      CALL DESORB
   19 ADT = DTMAX
      DO 60 N=1,NDX1,4
      ADT2=WI       /(ABS(W(NDR4,N)-WS(N))+1.E-9)*DT
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TS(N)-TS2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TX(N)-TX2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
      ADT2=TI/(ABS( TC(N)-TC2(N))+1.E-9)*DT*2.0
      IF(ADT2.LT. ADT) ADT=ADT2
   60 CONTINUE
      IF(ADT.LT. 1.E-5)ADT=1.E-5
      DTT(IBED)=ADT
      DO 21 N=1,NDX1
      TS2(N)=TS1(N)
      TS1(N)=TS(N)
      TX2(N)=TX1(N)
      TX1(N)=TX(N)
      TC2(N)=TC1(N)
      TC1(N)=TC(N)
   21 CONTINUE
      IF(IFLIP .NE. 0) CALL FLAP
      DO 211 N= 1, NDX1
  211 TOTKWH=TOTKWH+DT*HTR(N)/3410.
      TOTHTC=TOTHTC+WC*CPC(NOG)*DT*(T268-TC(NDX1))
      IF(
     1  ((TIME.LT.1.1E-5).OR.(TIME.GE.CYCLE).OR.  (NPR/NPRINT*NPRINT
     2.EQ.NPR)).AND. (NCYCLE.GE. NSTART))  GO TO 130
      GO TO 33
  130 CONTINUE
      GO TO(131,32) ,IAD
  131 CALL PRADSB(IBED)
      GO TO 33
   32 CALL PRDESB(IBED)
      GO TO 33
   33 DO 20 N=1,349
   20 RBM(N)=TG(N)
      DO 23 N=1,251
   23 RBAD(N)=HXG(N)
```

```
      DO 41 N= 1, 405
   41 RB(N)=ABED(N)
      DO 181 N=1,29
  181 IB(N)=NPSET(N)
      RETURN
   18 SUMCOS=0.
      IF(NDXM.EQ.NDX1)CALL EXIT
      NDB=NDXM+1
      DO 42 N=NDB,NDX1
      CALL EQPWT(1,IDSORB(N),2,3.,WN1,70.)
      WN(N)=WN1*ABED(N)*DX*RHOSB(N)
      SUMCOS=SUMCOS+WN(N)*FCOAD(IDSORB(N),W(1,N))
   42 CONTINUE
      DO 43 N=NDB,NDX1
      DIF(N)=DIF(1)
      GK(N)=GK(1)
      DH(N)=DH(1)
      IF(SUMCOS-WN(N))46,44,44
   46 CONTINUE
      FRHO=SUMCOS/WN(N)
      DRHO=RHOSB(N)*(1.-FRHO)
      RHOSB(N)= RHOSB(N)*FRHO
      IF(N.LT.NDX1) GO TO 51
      RHOSB(N+1)=DRHO
      GO TO 50
   51 NTDB=NDX1-N
      DRHO1=DRHO/NTDB
      K1=N+1
      DO 53 K=K1,NDX1
   53 RHOSB(K)=RHOSB(K)+DRHO1
   50 NDXM=N
      NDXMAC=N
      ASG(N)=ASG(1)*RHOSB(N)/RHOSB(1)
      IF(N.EQ.NDX1)NDX1=NDX1+1
      GO TO 47
   44 SUMCOS=SUMCOS-WN(N)
      ASG(N)=ASG(1)*RHOSB(N)/RHOSB(1)
      IF(SUMCOS.LT.1.E-10) GO TO 50
   43 CONTINUE
   47 CONTINUE
   49 CONTINUE
      ASSIGN 83 TO NPRSBR
      GO TO 183
   83 CONTINUE
      GO TO 33
   90 CONTINUE
      PK(1,1)=PCO2I
   91 PK(2,1)=PH2OI
      TG(1)=TGI
      GO TO 33
C
C
C  PRSBWT ROUTINE   CCCCCCCCCC
  183 CONTINUE
      WCC=WC
      N1=NDXM+1
      VMS = 0.0
      WTMS=0.0
      VSG=0.0
      WTSG=0.0
```

```
      IF(NDXM .EQ. 0) GO TO 11
      DO 10 N= 1, NDXM
      VMS=VMS+DX*ABED(N)
      WTMS=WTMS+DX*ABED(N)*RHOSB(N)
   10 CONTINUE
   11 CONTINUE
      IF((NDX1-NDXM) .EQ. 0) GO TO 31
      DO 30 N= N1,NDX1
      VSG=VSG+DX*ABED(N)
      WTSG=WTSG+DX*ABED(N)*RHOSB(N)
   30 CONTINUE
   31 CONTINUE
      WTACMS=0.0
      WN2L=0.0
      WO2L=0.0
      TN2=70.
      TO2=70.
      IF(NDXMAC .EQ. 0) GO TO 12
      DO 70 N= 1, NDXMAC
      CALL EQPWT(3,IDSORB(N),2,PN2,WN2,TN2)
      CALL EQPWT(4,IDSORB(N),2,PO2,WO2,TO2)
      WN2L=WN2L+DX*ABED(N)*RHOSB(N)*WN2
      WO2L=WO2L+DX*ABED(N)*RHOSB(N)*WO2
   70 WTACMS=WTACMS + DX*ABED(N)*RHOSB(N)
   12 CONTINUE
      WRITE(6,503) IBED
  503 FORMAT(1H1////7H BED NO I2////  20H VOLUME AND WEIGHT  //    )
      WRITE(6,500) VMS,WTMS,WTACMS,VSG,WTSG
  500 FORMAT(
     1' BULK VOLUME OF CO2 SORBENT (CU FT) 'F8.4/
     2' WEIGHT OF CO2 SORBENT (LB)         'F8.4/
     3' WEIGHT OF ACTIVE CO2 SORBENT (LB)  'F8.4//
     4' BULK VOLUME OF DESICCANT (CU FT)   'F8.4/
     5' WEIGHT OF DESICCANT (LB)           'F8.4)
C
      CALL START
      WN2V=0.
      WO2V=0.0
      DO 600 N=1,NDX1
      VOLN=ABED(N)*DX*VOIDF(N)
      WN2V=WN2V+28./359.*492./(70.+460.)/760.*PN2*VOLN
      WO2V=WO2V+32./359.*492./(70.+460.)/760.*PO2*VOLN
  600 CONTINUE
      WN2L=WN2L+WN2V
      WO2L=WO2L+WO2V
      RN2L=WN2L/CYCLE/2.0
      RO2L=WO2L/CYCLE/2.
      WRITE(6,505) RN2L,RO2L
  505 FORMAT(/////' ESTIMATED CABIN GAS LOSSES'//
     1' NITROGEN LOSS (LB/HR)              'F8.4/
     2' OXYGEN LOSS (LB/HR)                'F8.4)
      GO TO NPRSBR
      END
```

END CUR

```
@ ELT DESORB,1,710719, 62340   , 1
      SUBROUTINE DESORB
C
      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)          *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),           *NEW
     2TC2 (20),W (4,20),PT (20),        GMR ,GMW,GVIS, PN2,PO2,                   *NEW
     3               ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),            *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                      *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                           *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),                 *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                       *NEW
     8                                HXG(20),HXS(20),HXC(20),HSG(20),            *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,            *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                          *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,                   *NEW
     1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),          *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),            *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),             *NEW
     3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3         *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),          *NEW
     5              WM(2),TIME,CYCLE,DTO,   DTMAX,WI,TI,PCO2C,                    *NEW
     6VOLCAB,RCO2C,                                                               *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS               *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,                   *NEW
     1       CP1,CP2,X,   C1P,C2P,C3P,D1P                                         *NEW
      DIMENSION AS(20), PD(20)                                                    **-1
      DIMENSION P4(20),VIST(2)
      DOUBLE PRECISION G,DPKDTS,DPKDWK,PD
      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
     1,HGS)
      EQUIVALENCE (PS,P4)
      DIMENSION SPT(10), PET(10)
      EQUIVALENCE (SPT,VPUMP),(PET,PUMP)
      DATA VIST/0.014, 0.009/
      DATA RGAS/554./
C
      IF(TIME .LE.1.E-5)PF13=3.
      NDR=NDR4-1
      DO 21 N=1,NDX1
      J=2
      P4(N)=PT(N)
      AS(N)=4.*3.1416*RS(N)**2
      I=IFN(N,NDXM)
      IF( I .EQ. 2) J=1
      VIS= X(N)*VIST(I)+(1.-X(N))*VIST(J)
      F(N)=2.494E-4*PT(N)**0.795*(VIS/0.0174)
      DO 20 NR=1,NDR4
      I=N
      C1(NR,N)=-CR2(I,NR)
      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
   20 C3(NR,N)=-CR3(I,NR)
C
C
      B(1,N)=C3(1,N)/C2(1,N)
      DO 21 J=2,NDR
   21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
      NDX=NDX1-1
C     TO TEMPORARILY STORE SURFACE LOADING
      DO 50 N=1,NDX1
```

```
   50 WS(N)=W(NDR4,N)
C
C     TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
      IF (NTEMP .EQ. 0 ) GO TO 111
      DO 12 N=1,NDX1
      I=IFN(N,NDXM)
      CS2(N)=DT/CPS(N)/RHOSB(N)*ASG(N)*GK(N)*WM(I)*DH(N)
      CS1(N) = CS2(N)*X(N)
      IF (N.EQ.1) GO TO 13
      IF (N.EQ.NDX1) GO TO 14
      S1=SK(N)/DX**2*(TS(N-1)-2.*TS(N)+TS(N+1))
      GO TO 15
   13 S1=SK(1)/DX**2*(TS(2)-TS(1))
      GO TO 15
   14 S1=SK(NDX1)/DX**2*(TS(NDX)-TS(NDX1))
   15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+
     1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
      RATIO = (DT+DTO)/DT
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=RATIO*CS1(N)/(1.+T1)
      CS2(N)=RATIO*CS2(N)/(1.+T1)
      DS(N)=RATIO*DS(N)
      DS(N)= (DS(N)-T1*TS2(N))/(1.+T1)
   12 CONTINUE
      GO TO 110
  111 DO 112 N=1,NDX1
      CS1(N)=0.
      CS2(N)=0.
      DS(N)=0.
      TS(N)=T268
      TC(N)=T268
      TX(N)=T268
      TG(N)=T268
  112 CONTINUE
  110 CONTINUE
C
C     TO CALCULATE TOTAL PRESSURE
C
      DO 24 N=1,NDX1
      I=IFN(N,NDXM)
C     TO CALCULATE P1,P2,P3
      WSURF=W(NDR4,N)
      CALL EQPWT(I,IDSORB(N),1,PSURF,WSURF,TS2(N))
      CALL EQPWT(I,IDSORB(N),1,PS1,    WSURF,(TS2(N)+0.02))
      DPKDTS=(PS1-PSURF)/0.02
      CALL EQPWT(I,IDSORB(N),1,PS2,(WSURF+1.E-5),TS2(N))
      DPKDWK=(PS2-PSURF)/1.E-5
      G=1.+CS2(N)*DPKDTS
      P1(N)=(PSURF                    +DS(N)*DPKDTS)/G
      P2(N)=DPKDWK/G
      P3(N)=CS1(N)/G*DPKDTS
C
      C2(NDR4,N)=CR1(N,NDR4)/DT+CR2(N,NDR4)+WM(I)*GK(N)*P2(N)*AS(N)
      C3(NDR4,N)=0.0
      DO 23 NR=1,NDR4
   23 D1(NR,N)=CR1(N,NR)/DT*W(NR,N)
      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(N)
      D2(N)=AS(N)*WM(I)*GK(N)*(X(N)    -P3(N))
      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))
```

```
          Q(1,N)=D1(1,N)/C2(1,N)
          DO 24 J=2,NDR4
       24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
C
C         COEFFICIENTS FOR P-EQUATION
          DO 25 N=2,NDX
       25 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1
         1)/F(N+1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(2.*DX)
          N=1
          PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1
         1)/F(N+1) - VOIDF(N   )*C(N   )*ABED(N   )/F(N   ))/(1.*DX)
          N= NDX1
          PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N   )*C(N   )*ABED(N
         1)/F(N   ) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(1.*DX)
          DO 26 N=1,NDX1
          PC1(N)=PT(N)/F(N)
       26 PC3(N)=PT(N)/C(N)/VOIDF(N)*ASG(N)*GK(N)
C
          DO 27 N=1,NDX1
          CP1(N)=PC3(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
          CP2(N)=PC3(N)*(P2(N)*D2(N)+P3(N)      -X(N))
          C1P(N)=-PC1(N)/DX/DX+PC2(N)/2./DX
          C2P(N)=1./DT+2.*PC1(N)/DX/DX-CP2(N)
          C3P(N)=-PC1(N)/DX/DX-PC2(N)/2./DX
       27 D1P(N)=PT(N)/DT+CP1(N)
C
C         BOUNDARY CONDITION FOR P-EQUATION
C
          C2P(1)=C2P(1)+C1P(1)
          C1P(1)=0.
          GO TO (55,56,58,58), NBCOUT
       58 CONTINUE @  PUMP CHARACTERISTIC GIVEN
          POPI=PCO2A*51.7/PT(NDX1)
          CALL LAGIN2( 58,PUMP,10,2,POPI,VPUMP1,VPUMP)
          VPUMP1=VPUMP1*(TG(NDX1)+460.)/(TCO2A+460.)
          IF(VPUMP1 .LT. 0.0) VPUMP1=0.00
          CEXIT=VPUMP1*60./(ABED(NDX1)*VOIDF(NDX1))/PT(NDX1)
          GO TO 59
C
       55 CONTINUE
          EMW=X(NDX1)*WM(2)+(1.-X(NDX1))*WM(1)
          EVIS=X(NDX1)*VIST(2)+(1.-X(NDX1))*VIST(1)
          EVIS=EVIS*0.01
          SQTM= SQRT( (TG(NDX1)+460.)/1.8/EMW)
          DIA=6.0
          TOTL=127.
          PTAVG=0.5*(PT(NDX1)+PF13)
          EV=3.269E-2*PTAVG*    DIA**4/TOTL/EVIS+
         13.81*DIA**3/TOTL*(SQTM+0.147*PTAVG*    DIA/EVIS)
         2/(SQTM+0.181*PTAVG*    DIA/EVIS)
          EV=EV*3600./28.316
          EV1=EV
          N1=1
       91 CONTINUE
          QF=(PT(NDX1)-PF13)*EV
          CALL LAGIN2(58,PET,10,2,PF13,SP,SPT)
          DQF=QF-SP*PF13
          CALL NEWTO2(N1,NGO,PF13,DQF,PF130,DQFO,1.E-3,PT(NDX1),0,0111)
          GO TO (91,92), NGO
       92 CONTINUE
```


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```
      EV=SP*EV/(SP+EV)
      C2P(NDX1)=C2P(NDX1)+C3P(NDX1)*(1.-EV*F(NDX1)*DX/VOIDF(NDX1)/ABED
     1(NDX1)/PT(NDX1))
      C3P(NDX1)=0.000
      GO TO 57
C
   59 C2P(NDX1) = C2P(NDX1)+C3P(NDX1)*(1.-DX*F(NDX1)*CEXIT)
      C3P(NDX1)=0.0
      GO TO 57
   56 CONTINUE
C  PRESSURES ARE SET
C
      DO 561 K= 1, 3
      IF(NPSET(K) .EQ. 0) GO TO 561
      NP=NPSET(K)
      C1P(NP)=0.0
      C2P(NP)=1.0
      C3P(NP)=0.0
      CALL LAGIN2(10,TIMET,10,2,TIME,D1PNP   ,POUT)
      D1P(NP)=D1PNP
  561 CONTINUE
   57 CONTINUE
      CALL FDEQID(C1P,C2P,C3P,D1P,PD,NDX1)
      DO 34 N=1,NDX1
      IF(PD(N) .LE. 0.) PD(N) = 1.E-3
   34 PT(N)=PD(N)
C
C     TO CALCULATE SORBENT LOADING
C
      DO 30 N=1,NDX1
      W(NDR4,N)=Q(NDR4,N)+D2(N)*PT(N)
      DO 30 J=2,NDR4
      L=NDR4+1-J
   30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
C
C     TO CALCULATE STREAM COMPOSITION
C
      FR(1,1) = 0.0
      FR(2,1)=0.
      FR2=0.0
      DO 31 N=1,NDX1
      I=IFN(N,NDXM)
      TEMP   =C(N)*VOIDF(N)
     1/P4(N)*ABED(N)                 *DX*(CP1(N)+CP2(N)*PT(N))
      IF(I.EQ.1)J=2
      IF(I.EQ.2)J=1
      IF(N . EQ. 1) GO TO 200
      FR(J,N)=FR(J,N-1)
      FR(I,N)=TEMP+FR(I,N-1)
      IF( NDXM .EQ. 0) GO TO 202
      IF (I .EQ. 1) GO TO 202
      IF(NPSET(2) .NE. 0) GO TO 202
      GO TO 201
  200 FR(I,1) = TEMP
  202 X(N) = 1.0
      GO TO 31
  201 CONTINUE
      CT=ABED(N)*DX*ASG(N)*GK(N)
      FRT= FR(1,N)+FR(2,N)+1.E-10
      PSURF = P1(N)+P2(N)*(W(NDR4,N)-WS(N))+P3(N)*PT(N)
```

```
      X(N)=((FR(2,N-1)+CT*PSURF                               )/FRT/
     1 (1.+CT*PT(N)/FRT)      )
      IF(X(N) .LT. 0.0) X(N)=0.0
      IF(X(N) .GT. 1.0) X(N)=1.0
   31 CONTINUE
      DO 33 N=1,NDX1
      C(N) = (PT(N)/RGAS/(TG(N)+460)+C(N))/2.0
      I = IFN (N,NDXM)
      IF (I.EQ.1) J=2
      IF (I.EQ.2) J=1
      RHOG(N)=C(N)*(X(N)*WM(I)+(1.-X(N))*WM(J))
      UG(N)=(FR
     1        (1,N)*WM(1)+FR(2,N)*WM(2))/RHOG(N)/ABED(N)/VOIDF(N)
   33 CONTINUE
      IF( NTEMP .EQ. 0) RETURN
C
C     TO CALCULATE SORBENT TEMPERATURES
C
      CALL TSORB
      D9=DT
      CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,D9,
     1AVC, NOG   ,DTQ,TS1,TS2,TX1,TX2,TC1,TC2)
      CALL HXCORE
      CALL GAST(DX,RHOG,CPG,UG,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF)
  100 FORMAT(8G12.3)
      DESRAT=FR(1,NDX1)
      IF(NBCOUT .EQ. 3) GO TO 101
      IF(NBCOUT .EQ. 4) GO TO 1018
      RETURN
  101 CONTINUE
      DPCO2A=(DESRAT-SABCO2/44.)*DT*RGAS*(TCO2A+460.)/VCO2A/51.7
      PCO2A=PCO2A+DPCO2A
      RETURN
 1018 CONTINUE
      DVCO2A = (DESRAT -SABCO2/44.0)*DT*RGAS*(TCO2A+460.0)/PCO2A/51.7
      VCO2A=VCO2A+DVCO2A
      RETURN
      END
```

```
@ ELT EQPWT,1,710712, 56799     , 1
              SUBROUTINE EQPWT(ID,IDSORB,KPW,P,W,T)
      C     KPW=1   =  W,T    TO FIND P
      C     KPW=2  =      P,T    TO FIND W
      C      PKEQ=EQUILIBRIUM PRESSURE IN MM HG
      C      W=LOADING IN LB ADSORBATE PER LB ADSORBENT
      C      T=TEMP IN DEG F
      C
             DIMENSION TTAB(10,25), WTAB(15,10,25), PTAB(15,10,25), NT(25)
             DIMENSION IDSMTX(5,5)
      C  NT(1)  DATA  FOR   CO2  ON   MOL SIEVE  5A
      C  NT(2)  DATA  FOR   H2O  ON   MOL SIEVE  5A
      C  NT(3)  DATA  FOR   H2O  ON   SILICA GEL
      C  NT(4)  DATA  FOR   CO2  ON   MOL SIEVE  13X
      C  NT(5)  DATA  FOR  H2O  ON MOL SIEVE  13X
             DATA IDSMTX/1,0,4,0,0,2,3,5,  0,0, 6,0,8,0,0,7,0,9,0,0,0,0,0,0,0/
             DATA JACK/0/
             DATA NT/25*0./
      C
             DATA NT(1)/6/
             DATA (TTAB(J,1),J=1,6)/392.,212.,122.,77.,51.,32,/
             DATA (WTAB(I,1,1),I=1,15)/.001,.0018,.0021,.0025,.003,.0037,.004,
            1.0045,.005,.0055,.0063,.007,.008,.0088,.0092/
             DATA (PTAB(I,1,1),I=1,15)/1.0,1.5,2.0,2.5,3.0,4.0,5.0,7.0,8.0,10.,
            115.,20.,30.,40.,50./
             DATA (WTAB(I,2,1),I=1,15)/.002,.0028,.004,.0047,.0052,.006,.007,
            1.009,.01,.012,.015,.019,.025,.03,.034/
             DATA (PTAB(I,2,1),I=1,15)/1.0,1.5,2.0,2.5,3.0,4.0,5.0,7.0,8.0,10.,
            115.,20.,30.,40.,50./
             DATA (WTAB(I,3,1), I=1,15)/ 0.0009,0.0018,0.0025,0.0027,0.0043,
            10.0065,0.01,0.0145,0.0178,0.0265,0.0325,0.04,0.0485,0.057,0.07/
             DATA(WTAB(I,5,1),I=1,15)/0.002,0.005,0.008,0.0122,0.018,0.0255,
            10.0324.0.04,0.05,0.07,0.08,0.09,0.1,0.11,0.1177/
             DATA(WTAB(I,6,1),I=1,15)/0.0016,0.0035,0.0073,0.01,0.015,0.02,
            10.0277,0.04,0.05,0.06,0.077,0.09,0.1,0.11,0.12/
             DATA (PTAB(I,3,1),I=1,15)/.05,.1,.2,.3,.7,1.,1.9,3.,4.,7.,
            110.,14.5,20.,26.,40./
             DATA (WTAB(I,4,1),I=1,15)/.0009,.0025,.0033,.006,.0093,.013,
            10.0174,.027,.0347,.041,.05,.06,.08,.0955,.103/
             DATA (PTAB(I,4,1),I=1,15)/.03,.06,.1,.2,.4,.7,1.,2.,
            13.,4.,5.6,7.7,13.,20.,26.5/
             DATA (PTAB(I,5,1),I=1,15)/0.02,.05,.1,.2,.4,.7,1,,1.5,
            12.17,3.9,5.,7.,10.,15.,20./
             DATA (PTAB(I,6,1),I=1,15)/0.01,.03,.06,.1,.2,.3,.5,.88,
            11.32,1.8,3.,4.65,6.6,9.5,15./
      C
             DATA NT(2)/6/
             DATA (TTAB(J,2),J=1,6)/392.,212.,167.,122.,77.,32./
             DATA (WTAB(I,1,2),I=1,15)/.004,.007,.01,.012,.015,.018,.02,.023,
            1.028,.038,.05,.071,.076,.081,.09/
             DATA (PTAB(I,1,2),I=1,15)/.01,.02,.05,.1,.2,.5,1,,2.,5.,10.,20.,
            150.,60.,75.,100./
             DATA (WTAB(I,2,2),I=1,15)/.02,.024,.026,.030,.036,.045,.051,.058,
            1.074,.091,.11,.135,.15,.16,.175/
             DATA (PTAB(I,2,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1.0,2.0,
            14.0, 10., 20., 40., 100./
             DATA (WTAB(I,3,2),I=1,15)/.027,.035,.038,.045,.057,.071,.08,.092,
            1.11,.125,.135,.145,.16,.18,.19/
             DATA (PTAB(I,3,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1.,2.,3.,4.,
```

```
     110.,60.,120./
      DATA (WTAB(I,4,2),I=1,15)/.045,.058,.065,.078,.097,.115,.125,.135,
     1.145,.160,.165,.175,.180,.185,.188/
      DATA (PTAB(I,4,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1.,2.,3.,10.
     1,20.,60.,120./
      DATA (WTAB(I,5,2),I=1,15)/.083,.103,.115,.12,.14,.155,.159,.163,
     1.175,.18,.181,.182,.183,.184,.185/
      DATA (PTAB(I,5,2),I=1,15)/.01,.02,.03,.04,.1,.2,.3,.5,1.,2.,4.,7.,
     115.,40.,100./
      DATA(WTAB(I,6,2),I=1,15)/.135,.15,.155,.16,.167,.169,.173,.178,.18
     10,.181,.183,.184,.185,.186,.187/
      DATA (PTAB(I,6,2),I=1,15)/.01,.02,.03,.04,.07,.10,.20,.50,1.5,3.0,
     17.0,15.0,30.0,70.0,100.0/
C
      DATA NT(3)/5/
      DATA (TTAB(J,3),J=1,5)/160.,100.,60.,40.,10./
      DATA (WTAB(I,1,3),I=1,15)/.0018,.0026,.0031,.0057,.008,.01,.03,
     1.06,.10,.14,.20,.32,.45,.49,.50/
      DATA (PTAB(I,1,3),I=1,15)/.01,.05,.1,.4,1.0,1.95,9.42,23.6,44.8,
     167.2,101.8,200.,400.,700.,1000./
      DATA (WTAB(I,2,3),I=1,15)/.00305,.005,.0069,.009,.02,.05,.07,.11,
     1.17,.215,.32,.42,.50,.58,.59/
      DATA (PTAB(I,2,3),I=1,15)/.01,.05,.10,.2,.87,3.20,5.04,9.06,15.6,
     120.,30.,50.,100.,300.,700./
      DATA (WTAB(I,3,3),I=1,15)/.005,.008,.01,.02,.04,.05,.06,.10,.19,
     1.27,.405,.50,.55,.60,.64/
      DATA (PTAB(I,3,3),I=1,15)/.01,.03,.07,.206,.574,.79,1.02,2.04,4.7,
     17.23,15.,30.,50.,100.,300./
      DATA (WTAB(I,4,3),I=1,15)/.008,.0092,.01,.02,.03,.05,.07,.11,.27,
     1.40,.42,.48,.57,.67,.75/
      DATA (PTAB(I,4,3),I=1,15)/.01,.02,.03,.092,.17,.36,0.58,1.08,3.45,
     16.0,8.0,10.0,20.0,70.0,200.0/
      DATA (WTAB(I,5,3),I=1,15)/.014,.018,.022,.05,.08,.205,.28,.35,.42,
     1.50,.60,.70,.77,.80,.82/
      DATA (PTAB(I,5,3),I=1,15)/.01,.02,.03,.10,.20,.70,1.0,1.5,2.0,3.0,
     15.0,10.0,20.0,40.0,100.0/
C
      DATA NT(4)/3/
      DATA (TTAB(J,4),J=1,3)/122.,77.,32./
      DATA (WTAB(I,1,4),I=1,15)/.00355,.0036,.00365,.0037,.0038,.0040,
     1.0045,.005,.0059,.0077,.011,.016,.020,.026,.037/
      DATA (PTAB(I,1,4),I=1,15)/.02,.03,.04,.05,.07,.10,.20,.30,.50,1.0,
     12.0,4.0,6.0,10.0,20.0/
      DATA (WTAB(I,2,4),I=1,15)/.0098,.01,.0105,.0115,.0124,.0133,.0150,
     1.0165,.018,.021,.033,.0415,.0475,.055,.064/
      DATA (PTAB(I,2,4),I=1,15)/.025,.05,0.1,0.2,0.3,0.4,0.6,0.8,1.0,1.5
     1,4.0,7.0,10.0,15.0,25.0/
      DATA (WTAB(I,3,4),I=1,15)/.018,.0187,.0191, .02,.0222,.0248,.0282,
     1.031,.033,.0355,.04,.05,.068,.078,.095/
      DATA (PTAB(I,3,4),I=1,15)/.002,.01,.02,.04,.10,.20,.40,.60,.80,1.,
     11.5,3.0,6.0,10.0,20.0/
C
      DATA NT(5)/6/
      DATA (TTAB(J,5),J=1,6)/400.,300.,200.,122.,77.,35./
      DATA (WTAB(I,1,5),I=1,15)/.0001,.0002,.0005,.001,.002,.003,
     1.005,.01,.016,.022,.03,.041,.05,.06,.07/
      DATA (PTAB(I,1,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
     11.,2.,5.,10.,20.,50./
      DATA (WTAB(I,2,5),I=1,15)/.001,.002,.003,.004,.009,.012,.018,
     1.025,.038,.048,.06,.078,.09,.102,.118/
```

```
      DATA (PTAB(I,2,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
     11.,2.,5.,10.,20.,50./
      DATA (WTAB(I,3,5),I=1,15)/.007,.01,.015,.02,.026,.036,.046,.058,
     1.075,.09,.104,.124,.14,.153,.17/
      DATA (PTAB(I,3,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
     11.,2.,5.,10.,20.,50./
      DATA (WTAB(I,4,5),I=1,15)/.049,.052,.054,.059,.067,.083,.096,
     1.116,.132,.152,.164,.180,.196,.208,.225/
      DATA  (PTAB(I,4,5),I=1,15)/.001,.003,.005,.01,.02,.05,.09,.2,
     1.35,.72,1.013,2.22,4,65,8.5,20./
      DATA (WTAB(I,5,5),I=1,15)/.068,.072,.078,.090,.105,.124,.14,
     1.156,.165,.182,.196,.209,.224,.24,.256/
      DATA (PTAB(I,5,5),I=1,15)/.001,.003,.005,.01,.02,.05,.1,.2,.3,
     1.6,1.1,2.0,4.0,9.0,19./
      DATA (WTAB(I,6,5),I=1,15)/.108,.112,.13,.144,.158,.172,
     1.186,.198,.213,.224,.236,.252,.268,.28,.30/
      DATA (PTAB(I,6,5),I=1,15)/.001,.002,.005,.01,.02,.04,.08,.15,.3,
     1.5,.85,1.7,3.5,6.2,20./
C
      DATA NT(6)/3/
      DATA (TTAB(J,6), J=1,3)/120., 68., 32./
      DATA(PTAB(I,1,6),I=1,15) / 15., 20.,30.,40.,60.,80.,100.,125.,150.,
     1,200., 250.,350.,450.,600.,750./
      DATA(PTAB(I,2,6),I=1,15) / 15., 20.,30.,40.,60.,80.,100.,125.,150.,
     1,200., 250.,350.,450.,600.,750./
      DATA(PTAB(I,3,6),I=1,15) / 15., 20.,30.,40.,60.,80.,100.,125.,150.,
     1,200., 250.,350.,450.,600.,750./
      DATA (WTAB(I,1,6),I=1,15)/.0005,.0006,.0007, .0009,.00116,.00137,
     1.00155,.00178,.00205,.00250,.0031,.00435,.00565,.0073,.0087/
      DATA (WTAB(I,2,6),I=1,15)/.0007,.00078,.00102,.00126,.00173,
     1.00207,.0025,.0030,.00348,.0044,.0052,.0068,.0083,.0103,.0122/
      DATA (WTAB(I,3,6),I=1,15)/
     1.0012,.0014,.0019,.0023,.0030,.0037,.00435,.0052,.00602,
     2.0075,.0087,.01135,.0137,.0167, .0197/
      DATA NT(7)/2/
      DATA (TTAB(J,7),J=1,2)/70., 32./
      DATA (PTAB(I,1,  7),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (PTAB(I,2,  7),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (WTAB(I,1,7),I=1,15)/
     1.0002,.00025,.0003,.00043,.0005,.00065,.00082,.00105,.00125,.00146
     2,.00186,.00264,.0034,.0044,.00555/
      DATA (WTAB(I,2,7),I=1,15)/
     1.0002,.00025,.0003,.00044,.00056,.00073,.00096,.00122,.00148,
     2.00173,.00224,.00337,.00447,.00585,.0074/
      DATA NT(8)/3/
      DATA(TTAB(J,8),J=1,3)/120.,72.,32./
      DATA (PTAB(I,1,  8),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (PTAB(I,2,  8),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (PTAB(I,3,  8),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (WTAB(I,1,8),I=1,15)/
```

```
     1.0001,.0002,.0003,.0004,.0005,.0006,.00075,.0008,.001,.00115,
     2.0014,.002,.00255,.0035,.0047/
      DATA (WTAB(I,2,8),I=1,15)/
     1.00035,.0004,.00045,.0005,.0006,.0009,.0012,.00155,.0018,.0022,
     2.0028,.004,.0052,.0066,.0084/
      DATA (WTAB(I,3,8),I=1,15)/
     1.00065,.0007,.00085,.001,.0012,.0014,.0017,.0024,
     2.0032,.0036,.0050,.0069,.0085,.0108,.0144/
      DATA NT(9)/3/
      DATA (TTAB(J,9),J=1,3)/120.,72.,32./
      DATA (PTAB(I,1,  9),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (PTAB(I,2,  9),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (PTAB(I,3,  9),I=1,15)/
     110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
     2./
      DATA (WTAB(I,1,9),I=1,15)/
     1.0001,.00013,.00017,.0002,.00025,.0003,.00037,.00048,.00058,
     2.00067,.00087,.00122,.00163,.00221,.00291/
      DATA (WTAB(I,2,9),I=1,15)/
     1.0002,.00023,.00026,.00036,.00045,.00058,.0007,.00085,
     2.00099,.00111,.00136,.0019,.0024,.00312,.00396/
      DATA (WTAB(I,3,9),I=1,15)/
     1.00025,.00034,.00042,.00055,.00067,.00082,.001,.00122,
     2.00144,.00163,.00199,.00264,.00328,.0043,.00578/
C
      IF (W .LE. 0. ) W= 1.E-20
      IF(JACK .GT. 0) GO TO 102
      DO 105 K=1,25
      IF (NT(K) .EQ. 0) GO TO 90
      NTI=NT(K)
      DO 101 J=1,NTI
      TTAB(J,K)=1./(TTAB(J,K)+460.)
      DO 101 I=1,15
      WTAB(I,J,K)=ALOG(WTAB(I,J,K))
      PTAB(I,J,K)=ALOG(PTAB(I,J,K))
  101 CONTINUE
   90 CONTINUE
  105 CONTINUE
  102 CONTINUE
      IS=IDSMTX(IDSORB,ID)
      IF(IS.EQ.0) GO TO 999
      JACK = JACK + 1
      RT=1./(T+460.)
      GO TO (201,202), KPW
  201 WL=ALOG(W)
      N=NT(IS)
      PKEQ1=XYZMAP(1,WTAB(1,1,IS), PTAB(1,1,IS),15,TTAB(1,IS),N ,2,2,WL,
     1RT,ANS)
      P    =EXP(PKEQ1)
      IF (PKEQ .LT. 0.0) PKEQ=0.0
      RETURN
  202 PL=ALOG(P)
      N=NT(IS)
      W01=XYZMAP(1,PTAB(1,1,IS),WTAB(1,1,IS),15,TTAB(1,IS),N,2,2,PL,RT,
     1ANS)
      W=EXP(W01)

      RETURN
  999 WRITE(6,998) IDSORB,ID
  998 FORMAT(/////' EQUILIBRIUM DATA UNAVAILABLE FOR'/' IDSORB ='I4/'
     1  ID =' I4)
      CALL EXIT
      END
```

```
@ ELT FCOAD,1,710712, 56800     , 1

              FUNCTION FCOAD(IDSORB,H2O)
C
C
              DIMENSION H2OT(12), FCOADT(12,5)
              DATA H2CT/  0.00, .01, .02, .03, .04, .05, .06, ,07, .08, .10,
             1.12, .60/
              DATA (FCOADT(I,1),I=1,12)/1.,.98,.88,.72,.575, .436, .313, .22,
             1.155, .086, .055, .0/
              DATA(FCCADT(I,3),I=1,12)/1., .794, .63, .503, .415, .35, .298,
             1.252, .214, .148, .085, .0/
              CALL LAGIN2(666, H2OT          ,12,2,H2O,FCOAD,FCOADT(1,IDSORB))
              RETURN
              END
```

```
@ ELT FDEQID,1,710514, 38495    , 1

              SUBROUTINE FDEQID(C1,C2,C3,D,VAR,NN)
              DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
              DOUBLE PRECISION C1,C2,C3,D,VAR,B,Q
              NN1=NN-1
              B(1)=C3(1)/C2(1)
              DO 41 J=2,NN1
           41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
              Q(1)=D(1)/C2(1)
              DO 42 J=2,NN
           42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
              VAR(NN)=Q(NN)
              DO 43 J=2,NN
              L=NN+1-J
           43 VAR(L)=Q(L)-B(L)*VAR(L+1)
              RETURN
               END
```

```
@ ELT FDEQIM,1,710514, 38492    , 1

              SUBROUTINE FDEQIM(C1,C2,C3,D,VAR,NN)
              DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
              NN1=NN-1
              B(1)=C3(1)/C2(1)
              DO 41 J=2,NN1
           41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
              Q(1)=D(1)/C2(1)
              DO 42 J=2,NN
           42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
              VAR(NN)=Q(NN)
              DO 43 J=2,NN
              L=NN+1-J
           43 VAR(L)=Q(L)-B(L)*VAR(L+1)
              RETURN
              END
```

```
@ ELT FLAP,1,710719, 62342      , 1
      SUBROUTINE FLAP
      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,       PK (2,20),PCO2I  ,TS  (20)          *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),           *NEW
     2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,PO2,                 *NEW
     3              ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),             *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                      *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                           *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),                 *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                       *NEW
     8                            HXG(20),HXS(20),HXC(20),HSG(20),                *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,            *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX;                                          *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,                   *NEW
     1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),          *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),            *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),             *NEW
     3FR(2,20),        P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3        *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),          *NEW
     5              WM(2),TIME,CYCLE,DTO,    DTMAX,WI,TI,PCO2C,                   *NEW
     6VOLCAB,RCO2C,                                                               *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS               *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,                   *NEW
     1        CP1,CP2,X,    C1P,C2P,C3P,D1P                                       *NEW
      DIMENSION DUMMY(20),DUMM1(20),IDUMMY(20)                                    **-1
      NAMELIST /CHECK/
     1TG,PH2OI,TGI,PA,PK,PCO2I,TS,TC,TX,TS1,TS2,TX1,TX2,TC1,TC2,W,PT,
     2GMR,GMW,ABED,AVC,ASG,ASX,AGX,AXC, AVX,RHOG,RHOSB,RHOS,RHOC,RHOX,CP
     3G, CPC,CPX,CPS,DX,POUT,TIMET,WTACMS,WTSG,PUMP,VPUMP,NPSET,NDR4,
     4NDXMAC,NBCOUT,NDX1,NDXM,NOG,HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,UC,T2
     568, TOTCO2,TOTH2O,SUMPTM,AVMSL1,AVSGL1,HTR,TMAX,A,F,C,VS,DVS,DVS1
      CALL FLIP(W,TG,TS,TX,TC,NDX1,NDR4,NOG,UC)
      CALL FLOP(ABED,AVC,ASG,ASX,AGX,NDX1)
      CALL FLOP(AXC,AVX,RHOG,RHOSB,RHOC,NDX1)
      CALL FLOP(RHOX,CPG,CPC,CPX,CPS,NDX1)
      CALL FLOP(HXG,HXS,HXC,HSG,DH,NDX1)
      CALL FLOP(DIF,GK,PT    ,X     ,HTR   ,NDX1)
      CALL FLOP (TS1,DUMMY,DUMMY,DUMMY,DUMMY,NDX1)
      CALL FLOP(TS2,TX1,TX2,TC1,TC2,NDX1)
      NDX2=NDX1+1
      CALL FLOP(SK,TKX,DUMMY,DUMMY,DUMMY,NDX2)
      DO 61 K=1,2
      DO 62 N=1, NDX1
      DUMM1(N)=FR(K,N)
   62 DUMMY(N)=PK(K,N)
      DO 61 N=1,NDX1
      I=NDX1+1-N
      FR(K,I)=DUMM1(N)
   61 PK(K,I)=DUMMY(N)
      DO 63 N=1,NDX1
   63 IDUMMY(N)=IDSORB(N)
      DO 64 N=1,NDX1
      I=NDX1+1-N
   64 IDSORB(I)=IDUMMY(N)
      RETURN
      END
```


AIRESEARCH MANUFACTURING COMPANY
Los Angeles, California

```
@ ELT FLIP,1,710514, 38498      , 1
      SUBROUTINE FLIP(W,TG,TS,TX,TC,NX,NR,NOG,UC)
C     THIS SUBROUTINE INVERTS BED LOADINGS AND TEMPERATURES
      DIMENSION W( 4,20),TG(20),TS(20),TX(20),TC(20),UC(20)
      DIMENSION TW( 4,20),TTG(20),TTS(20),TTX(20),TTC(20),TUC(20)
      DO 5 I=1,NX
      DO 6 J=1,NR
    6 TW(J,I)=W(J,I)
      TTC(I)=TC(I)
      TTG(I)=TG(I)
      TTS(I)=TS(I)
      TTX(I)=TX(I)
    5 TUC(I)=UC(I)
      DO 10 N=1,NX
      I=NX+1-N
      DO 15 J=1,NR
   15 W(J,I)=TW(J,N)
      TG(I)=TTG(N)
      TS(I)=TTS(N)
      TX(I)=TTX(N)
      TC(I)=TTC(N)
   10 UC(I)=-TUC(N)
      NOG=NX+1-NOG
      RETURN
      END
```

```
@ ELT FLOP,1,710514, 38499      , 1
      SUBROUTINE FLOP(A,B,C,D,E,NX)
      DIMENSION A(41),B(41),C(41),D(41),E(41)
      DIMENSION AA(20),BB(20),CC(20),DD(20),EE(20)
      DO 10 I=1,NX
      AA(I)=A(I)
      BB(I)=B(I)
      CC(I)=C(I)
      DD(I)=D(I)
   10 EE(I)=E(I)
      DO 20 N=1,NX
      I=NX+1-N
      A(I)=AA(N)
      B(I)=BB(N)
      C(I)=CC(N)
      D(I)=DD(N)
   20 E(I)=EE(N)
      RETURN
      END
```

```
@ ELT GAST,1,710514, 38500      , 1
      SUBROUTINE GAST (DX,RHOG,CPG,U,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF
     1)
      DIMENSION RHOG(1),CPG(1),U(1),TS(1),TX(1),TG(1),ASG(1),HSG(1),HXG(
     11),VOIDF(1),AXG(1)
      W=1.0
      N2= NDX1-1
      TG(1)=TS(1)
      DO 10 N= 1, N2
      F= 0.5*(VOIDF(N)+ VOIDF(N+1))
      AS1=ASG(N+1)
      HS1=HSG(N+1)
      AX1=AXG(N+1)
      HX1=HXG(N+1)
      CP1=CPG(N)
      RO = 0.5*(RHOG(N)+RHOG(N+1))
      U1= 0.5*( U(N)+U(N+1))
      TS1=TS(N+1)
      TX1=TX(N+1)
      C1=1./(F*RO*CP1*U1)
      D=C1*(AS1*HS1*TS1+AX1*HX1*TX1)
      A=(AS1*HS1+AX1*HX1)*C1
   10 TG(N+1)=((1./DX-A*(1.-W))*TG(N)+D)/(1./DX+A*W)
      RETURN
      END
```

@ ELT GASTA,1,710514, 38501 , 1

```
      SUBROUTINE GASTA(GMR,CPG,ABED,NDX1,TGI,ASG,HSG,AXG,HXG,DX,TG,TS,TX
     1)
C
C     GAS TEMPERATURE CALCULATIONS FOR ADSORPTION
C
      DIMENSION CPG(1),ASG(1),HSG(1),HXG(1),TG(1),TS(1),TX(1),ABED(1),
     1AXG(1)
C
      TG(NDX1+1) = TGI
      DO 10 N=1,NDX1
      C=GMR*CPG(N)/ABED(N)
      N1=NDX1+1-N
      C1=ASG(N1)*HSG(N1)+AXG(N1)*HXG(N1)
   10 TG(N1) = (TG(N1+1)/DX+(ASG(N1)*HSG(N1)*TS(N1)+AXG(N1)
     1                                                *HXG(N1)*TX(N1))/
     1C)/(1./DX+C1/C)
      RETURN
      END
```

@ ELT HXCORE,1,710719, 62343 , 1

```
      SUBROUTINE HXCORE
      COMMON/AD/ TG(20),PH20I ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)          *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),           *NEW
     2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,PO2,                 *NEW
     3                ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),           *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                      *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                           *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),                 *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                       *NEW
     8                                HXG(20),HXS(20),HXC(20),HSG(20),            *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,            *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                          *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,                   *NEW
     1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),          *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),            *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),             *NEW
     3FR(2,20),        P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3        *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),          *NEW
     5               WM(2),TIME,CYCLE,DTO,    DTMAX,WI,TI,PCO2C,                  *NEW
     6VOLCAB,RCO2C,                                                               *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS               *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,                   *NEW
     1        CP1,CP2,X,    C1P,C2P,C3P,D1P                                       *NEW
      EQUIVALENCE (NDX,NDX1)                                                      **-1
      DIMENSION S1(20),S2(20),S3(20),DD(20)
C
      DN=DT+DTO
      DO 10 N=1,NDX
      T1= AVX(N)*(HXC(N)+HXS(N)+HXG(N))*0.5
      S1(N)=-TKX(N)/DX/DX
      S3(N)= -TKX(N+1)/DX/DX
      S2(N)= RHOX(N)*CPX(N)/DN -S1(N) - S3(N) + T1
   10 DD(N) = RHOX(N)*CPX(N)/DN*TX2(N) + AVX(N)*(HXC(N)
     1*TC1(N) + HXS(N)*TS1(N)+HXG(N)*TG(N)) - T1*TX2(N)+HTR(N)/(ABED(N)*
     2ASX(N)/AVX(N)*DX)
      S2(1)=S2(1)+S1(1)
      S1(1)=0.
      S2(NDX)=S2(NDX)+S3(NDX)
      S3(NDX)=0.D
      CALL FDEQIM(S1,S2,S3,DD,TX,NDX)
      RETURN
      END
```

@ ELT IFN,1,710514, 38502 , 1

```
      FUNCTION IFN(N,NDXM)
      IFN=1
      IF(N.GT.NDXM)IFN=2
      RETURN
      END
C
```

```
@ ELT LAGIN2,1,710514, 38503   , 1

      SUBROUTINE  LAGIN2(ID,X,NP,ND,XO,YO,Y)
C     REVISED FOR FORTRAN IV 8-8-65  S. WONG
      DIMENSION  X(2),  Y(2)
C
      ILO=1
      IF(XO-X(1))10,16,4
    4 IF(XO-X(NP))19,13,7
    7 ILO=NP-1
   10 IHI=ILO+1
      GO TO 46
   13 ILO=NP
   16 YO=Y(ILO)
      RETURN
   19 DO 22 ILO=2,NP
      IF(XO-X(ILO))25,16,22
   22 CONTINUE
   25 IHI=ILO
      ILO=IHI-1
      IF(ND-2)46,46,28
   28 DO 43 I=3,ND
      IF(ILO-1)40,40,31
   31 IF(IHI-NP)34,37,37
   34 IF (2.*XO-X(ILO-1)-X(IHI+1)) 37,37,40
   37 ILO=ILO-1
      GO TO 43
   40 IHI=IHI+1
   43 CONTINUE
   46 YO=0.0
      PN=1.0
      DO 49 I=ILO,IHI
   49 PN=PN*(XO-X(I))
      DO 58 I=ILO,IHI
      P=PN/(XO-X(I))
      DO 55 J=ILO,IHI
      IF(J-I)52,55,52
   52 P=P/(X(I)-X(J))
   55 CONTINUE
      YO=YO+P*Y(I)
   58 CONTINUE
      RETURN
    1 FORMAT (97X,7HLAGIN2 ,I4,E12.5)
      END
```

```
@ ELT MAIN4B,1,710719, 62345    , 1

      C  MAIN PROGRAM FOR ANALYZING 4-BED  SYSTEM FOR CO2 RECOVERY
      C
            COMMON/AD/ TG(20),PH20I ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)    *NEW
           1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),     *NEW
           2TC2 (20),W (4,20),PT (20),        GMR ,GMW,GVIS, PN2,PO2,             *NEW
           3                 ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),    *NEW
           4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                *NEW
           5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                     *NEW
           6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),           *NEW
           7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                 *NEW
           8                              HXG(20),HXS(20),HXC(20),HSG(20),        *NEW
           9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,      *NEW
           1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                    *NEW
           1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,             *NEW
           1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),    *NEW
           1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
           2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),       *NEW
           3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3   *NEW
           4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),    *NEW
           5            WM(2),TIME,CYCLE,DTO,   DTMAX,WI,TI,PCO2C,                *NEW
           6VOLCAB,RCO2C,                                                         *NEW
           7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS         *NEW
            DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,             *NEW
           1       CP1,CP2,X,   C1P,C2P,C3P,D1P                                   *NEW
            COMMON    TG1(20),PH20I1,TGI1,PA1,       PK1(2,20),PCO2I1 ,TS01(20)   **-1
           1,TC01(20),TX01(20), TS11(20),TS21(20),TX11(20),TX21(20),TC11(20),
           2TC21(20),W1(4,20),PT1(20),          GMR1,GMW1,GVIS1,PN21,PO21
            COMMON    TG2(20),PH20I2,TGI2,PA2,       PK2(2,20),PCO2I2 ,TS02(20)
           1,TC02(20),TX02(20), TS12(20),TS22(20),TX12(20),TX22(20),TC12(20),
           2TC22(20),W2(4,20),PT2(20),          GMR2,GMW2,GVIS2,PN22,PO22
            COMMON    TG3(20),PH20I3,TGI3,PA3,       PK3(2,20),PCO2I3 ,TS03(20)
           1,TC03(20),TX03(20), TS13(20),TS23(20),TX13(20),TX23(20),TC13(20),
           2TC23(20),W3(4,20),PT3(20),          GMR3,GMW3,GVIS3,PN23,PO23
            COMMON    TG4(20),PH20I4,TGI4,PA4,       PK4(2,20),PCO2I4 ,TS04(20)
           1,TC04(20),TX04(20), TS14(20),TS24(20),TX14(20),TX24(20),TC14(20),
           2TC24(20),W4(4,20),PT4(20),          GMR4,GMW4,GVIS4,PN24,PO24
            COMMON/B1/ RDB(405),IDB(29)
            COMMON/B2/RMB(405),IMB(29)
            COMMON/B1A/RDBA(260)
            COMMON/B1D/RDBD(260)
            COMMON/B2A/ RMBA(260)
            COMMON/B2D/ RMBD(260)
            DIMENSION  RB1M(349),RB2M(349),RB3M(349),RB4M(349),RMAIN(11),
           1IMAIN(06),KBED(4)
            EQUIVALENCE (RB1M(1),TG1(1)),(RB2M(1),TG2(1)),(RB3M(1),TG3(1)),
           1(RB4M(1),TG4(1)),(RMAIN(1),WM(1)),(IMAIN(1),NCYCLT)
            NAMELIST/MAIN/ WM, CYCLE,DTMAX,WI,TI,PCO2C,VOLCAB,RCO2C,
           1NPRINT,NDTCON,NTEMP,        TGC,PAC,PH20C,TGHX
           2,PCO2A,VCO2A,SABCO2,TCO2A,KBED,TIMEDS, NCT1, NST1, NCT2, NST2
            NAMELIST/B1M/                           PA1,      TS01,TC01,TX01,W1,
           1GMR1,GMW1,      PN21,PO21
            NAMELIST/B2M/                           PA2,      TS02,TC02,TX02,W2,
           1GMR2,GMW2,      PN22,PO22
            NAMELIST/B3M/                           PA3,      TS03,TC03,TX03,W3,
           1GMR3,GMW3,      PN23,PO23
            NAMELIST/B4M/                           PA4,      TS04,TC04,TX04,W4,
           1GMR4,GMW4,      PN24,PO24
            DATA PT2,PT4/ 40*3.0/,X/20*1./,C/20*0.2E-3/
```

```
      DATA DTT/4*1./
    1 CONTINUE                      @ TO READ IN DATA FOR A NEW PROBLEM
  108 FORMAT(13A6,A2)
  109 FORMAT(20X,13A6,A2)
      READ(5,MAIN)
      WRITE(6,MAIN)
      READ(5,B1M)
      WRITE(6,B1M)
      READ(5,B2M)
      WRITE(6,B2M)
      READ(5,B3M)
      WRITE(6,B3M)
      READ(5,B4M)
      WRITE(6,B4M)
      CALL READ1
      CALL READ2
      CALL READ3
      CALL READ4
      SABCOS=SABCO2
      NHALF=1
      DO 102 N= 1, 20
      TC11(N)=TC01(N)
      TC21(N)=TC01(N)
      TX11(N)=TX01(N)
      TX21(N)=TX01(N)
      TS11(N)=TS01(N)
      TS21(N)=TS01(N)
      TC12(N)=TC02(N)
      TC22(N)=TC02(N)
      TX12(N)=TX02(N)
      TX22(N)=TX02(N)
      TS12(N)=TS02(N)
      TS22(N)=TS02(N)
      TC13(N)=TC03(N)
      TC23(N)=TC03(N)
      TX13(N)=TX03(N)
      TX23(N)=TX03(N)
      TS13(N)=TS03(N)
      TS23(N)=TS03(N)
      TC14(N)=TC04(N)
      TC24(N)=TC04(N)
      TX14(N)=TX04(N)
      TX24(N)=TX04(N)
      TS14(N)=TS04(N)
      TS24(N)=TS04(N)
  102 CONTINUE
      NCYCLT=NCT1
      NSTART=NST1
      ASSIGN 103 TO NSUB4B
      GO TO 104
  103 CONTINUE
      CALL BED4(1,0,3,RB1M,RDB,IDB,RDBA,ISTOPC,KBED)
      CALL BED4(2,0,3,RB2M,RMB,IMB,RMBA, ISTOPC,KBED)
      DO 201 K=1,60
      N=K+120
      RMBD(N)=RMBA(N)
      RDBD(N)=RDBA(N)
  201 CONTINUE
      NCYCLT=NCT2
      NSTART=NST2
```

```
      ASSIGN 105 TO NSUB4B
      GO TO 104
  105 CONTINUE
      CALL EXIT
C
C
  104 CONTINUE
C   START SUB4B
      NCYCLE=1
  101 CONTINUE
      IF(NCYCLE .GT. NCYCLT) GO TO NSUB4B
      TIME = 0.0
      DTO =0.0
      DT=1.E-5
      NPR = 1
      GO TO 3
    4 CONTINUE
      GO TO ( 3,42),NDTCON
   42 DT=DTMAX/10.0
      IF(TIME .LT. 1.E-4) DT=DTMAX/1000.0
      IF(TIME .GT. 0.06) DT=DTMAX
      GO TO 5
    3 CONTINUE
      DT=AMIN1(DTT(1),DTT(2),DTT(3),DTT(4))
      IF(TIME .LT. 8.E-5) DT=1.E-5
    5 IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
      TIME=TIME+DT
      GO TO(20,21), NHALF
C ********PART TO BE CHANGED FOR DIFFERENT HOOK-UP OF SYSTEM ******************
C  FIRST HALF CYCLE
   20 CONTINUE
      PCO2I1=PCO2C
      PH2OI1=PH2OC
      TGI1=TGC
      ISTOPC=0
      CALL BED4(1,0,1,RB1M,RDB,IDB,RDBA,ISTOPC,KBED)
      PCO2I2=PK (1,1)
      PH2OI2=PK (2,1)
      TGI2=TG (1)
      IF(TG1(1) .GT. TGHX) TGI2=TGHX
      RMBA(201)=TC01(10)
   35 CALL BED4(2,0,1,RB2M,RMB,IMB,RMBA,ISTOPC,KBED)
      DPCO2C=DT*(RCO2C-GMR*(PCO2C-PK2(1,1))*44./    (PA*GMW))*554.*530./
     1(44.*VOLCAB)
      IF((KBED(1).EQ.0),AND.(KBED(2).EQ.0))DPCO2C=0.
      PCO2C=PCO2C+DPCO2C
      PCO2I3=PK (1,1)
      PH2OI3=0.00000
      TGI3=TG (1)
      IF(TIME.GT.TIMEDS) ISTOPC=1
      CALL BED4(3,1,1,RB3M,RDB,IDB,RDBD,ISTOPC,KBED)
      RMBD(201)=TC03(10)
      CALL BED4(4,0,2,RB4M,RMB,IMB,RMBD,ISTOPC,KBED)
C ************************** TO BE CHANGED UP TO HERE ************************
      NPR = NPR+1
      DTO=DT
      IF(TIME .GE. CYCLE) NHALF=2
      IF(TIME .GE. CYCLE) GO TO 101
      GO TO 4
C ********PART TO BE CHANGED FOR DIFFERENT HOOK-UP OF SYSTEM ******************
```

```
C  SECOND HALF CYCLE
 21 CONTINUE
    ISTOPC=0
    PCO2I3=PCO2C
    PH2OI3=PH2OC
    TGI3=TGC
    CALL BED4(3,0,1,RB3M,RDB,IDB,RDBA,ISTOPC,KBED)
    PCO2I4=PK (1,1)
    PH2OI4=PK (2,1)
    TGI4=TG (1)
    IF(TG3(1) .GT. TGHX) TGI4=TGHX
    RMBA(201)=TC03(10)
 36 CALL BED4(4,0,1,RB4M,RMB,IMB,RMBA,ISTOPC,KBED)
    DPCO2C=DT*(RCO2C-GMR*(PCO2C-PK4(1,1))*44./    (PA*GMW))*554.*530./
   1(44.*VOLCAB)
    IF((KBED(3).EQ.0),AND.(KBED(4).EQ.0))DPCO2C=0.
    PCO2C=PCO2C+DPCO2C
    PCO2I1=PK (1,1)
    PH2OI1=0.0000
    TGI1=TG (1)
    IF(TIME.GT.TIMEDS) ISTOPC=1
    CALL BED4(1,1,1,RB1M,RDB,IDB,RDBD,ISTOPC,KBED)
    RMBD(201)=TC01(10)
    CALL BED4(2,0,2,RB2M,RMB,IMB,RMBD,ISTOPC,KBED)
C ************************** TO BE CHANGED UP TO HERE *************************
    NPR = NPR+1
    DTO=DT
    IF(TIME .GE. CYCLE) NHALF=1
    IF(TIME.GE.CYCLE) NCYCLE=NCYCLE+1
    IF(TIME.GE. CYCLE) GO TO 101
    GO TO 4
    END
```

```
@ ELT NEWTO2,1,710609, 32711   , 1
      SUBROUTINE NEWTO2(N1,NGO,X,Y,XO,YO,XMIN,XMAX,ER)
C     SET N1=1 IN MAIN PROGRAM BEFORE CALL NEWTON.  THE ROUTINE
C     FINDS X FOR Y=0  GIVES NGO=1 IF RECALCULATIONS REQUIRED.
C     GIVES NGO=2 IF CONVERGENCE REACHED.
      N1=N1-1
      IF( ABS(Y)-ER) 8,8,5
    5 IF(N1)7,6,7
    6 YO=Y
      XO=X
      X=XO+(XMAX-XMIN)*0.01
      IF(X-XMAX)21,21,14
   14 X=XO-(XMAX-XMIN)*0.01
      GO TO 21
    7 SLOPE=(Y-YO)/(X-XO)
      YO=Y
      XO=X
      X=X-Y/SLOPE
      IF(N1+8)20,20,21
   20 X=0.5*(X+XO)
      IF(N1+20)22,22,21
   22 WRITE (6,23)
      WRITE (6,30) X,Y,XO,YO,ER
   23 FORMAT (32HOEXCEED 20 ITERATIONS IN NEWTON //)
      N1=0
      ER=5.*ER
   21 CONTINUE
      IF(X-XMIN)11,11,12
   11 X=XMIN
      IF(X-XO)9,8,9
   12 IF(X-XMAX)9,13,13
   13 X=XMAX
      IF(X-XO)9,8,9
    9 NGO=1
      RETURN
    8 NGO=2
      N1=1
      RETURN
   30 FORMAT(14H X,Y,XO,YO,ER= 5G14.4)
      END
```


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```
@ ELT PRADSB,1,710719, 62347   , 1
      SUBROUTINE PRADSB(IBED)
C
      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)    *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),     *NEW
     2TC2 (20),W (4,20),PT (20),        GMR ,GMW,GVIS, PN2,PO2,              *NEW
     3                ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),      *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                 *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                       *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),            *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                  *NEW
     8                             HXG(20),HXS(20),HXC(20),HSG(20),          *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,        *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                      *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,               *NEW
     1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),       *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),        *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),         *NEW
     3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3     *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),      *NEW
     5              WM(2),TIME,CYCLE,DTO,    DTMAX,WI,TI,PCO2C,               *NEW
     6VOLCAB,RCO2C,                                                           *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS           *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,               *NEW
     1         CP1,CP2,X,    C1P,C2P,C3P,D1P                                  *NEW
C                                                                             **-1
      DIMENSION AVLD(41)
      EQUIVALENCE(NDX,NDX1)
      AVMSLD=0.0
      AVSGLD=0.0
      AVRCO2=0.0
      AVRH2O=0.0
      AVPH2O = SUMPTM/TIME
      AVH2OP=GMR*AVPH2O*18./(PA*GMW)
C
      TIMEM=60.*TIME
      WRITE(6,499)IBED
      WRITE(6,100) NCYCLE,TIME ,TIMEM,DT
      WRITE (6,101)
      WRITE(6,102)(N,PK(1,N),PK(2,N),
     1                    TG(N),TS(N),TC(N),TX(N),N=1,NDX)
      WRITE(6,103)PK(1,NDX1+1),PK(2,NDX1+1),TG(NDX1+1)
  103 FORMAT('        INLET' F10.4,F12.4,F19.4)
      WRITE (6,202)
      N1=NDXM+1
      NDR3=NDR4-1
      DO 20 N= 1, NDXM
      SUMMS=0.0
      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
      IF(NDR4.EQ.2) AVLD(N) = SUMMS
      IF(NDR4.EQ.2) GO TO 20
      DO 22 NR=2,NDR3
   22 SUMMS=SUMMS+W(NR,N)
      AVLD(N)=SUMMS/NDR3
   20 CONTINUE
      DO 30 N= N1,NDX1
      SUMMS=0.0
      SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
      IF(NDR4.EQ.2) AVLD(N) = SUMMS
```


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```
      IF(NDR4.EQ.2) GO TO 30
      DO 33 NR=2, NDR3
   33 SUMMS=SUMMS+W(NR,N)
      AVLD(N)=SUMMS/NDR3
   30 CONTINUE
      SUM=0.
      IF(NDXMAC .EQ. 0) GO TO 35
      DO 31 N= 1, NDXMAC
   31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVMSLD = SUM/WTACMS
      SUM=0.
   35 CONTINUE
      IF((NDX1-NDXM) .EQ. 0) GO TO 40
      DO 32 N= N1,NDX1
   32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVSGLD=SUM/WTSG
   40 CONTINUE
      DO 10 N=1,NDX
   10 WRITE (6,203)N, AVLD(N)
     1                ,(W(NR,N),NR=1,NDR4)
      IF(TIME .LT. 1.1E-5) AVMSL1=AVMSLD
      IF(TIME .LT. 1.1E-5) AVSGL1=AVSGLD
      AVRCO2=WTACMS*(AVMSLD-AVMSL1)/TIME
      AVRH2O=WTSG*(AVSGLD-AVSGL1)/TIME
C
      DIMENSION F1(9),F2(9),F3(9),F4(9),  F5(9),F6(9),F7(9)
      WRITE(6,205) F1,AVMSLD,F2,AVSGLD,F3,AVRCO2,F4,AVRH2O,F5,TOTKWH,
     1F6,TOTHTC,F7,AVPH2O
  205 FORMAT(////(9A6,F8.4,6X,9A6,F8.4 ))
      DATA F1/' AVG CO2 LOADING IN CO2 SORBENT (LB/LB)'/
      DATA F2/' AVG H2O LOADING IN DESICCANT (LB/LB)'/
      DATA F3/' TIME AVG CO2 ADSORPTION RATE (LB/HR)'/
      DATA F4/' TIME AVG H2O ADSORPTION RATE (LB/HR)'/
      DATA F5/' ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)'/
      DATA F6/' HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)'/
      DATA F7/' TIME AVG OUTLET PH2O (MM)'/
C
      RETURN
  499 FORMAT(8H1BED NO.  I3)
  100 FORMAT (1H0,16HADSORPTION CYCLE  I3/
     1          3X,5HTIME=,F9.5,1X2HHR,F12.3,1X,3HMIN,
     1                                   5X,15HTIME INCREMENT=F7.5,1X2HHR)
  101 FORMAT (//2X,10HAXIAL NODE,3X,7HPCO2,MM,5X,7HPH2O,MM,8X,
     1                                                     11HGAS TEMP, F
     1    ,8X,15HSORBENT TEMP, F     ,6X,15HCOOLANT TEMP, F    ,7X,15HHX CO
     2RE TEMP, F   )
  102 FORMAT(/(I9,2F12.4,5X,4(F14.4,6X)))
  202 FORMAT (//  38HOLOADING AT INTERIOR OF SORBENT, LB/LB
     1                                                 //4X,4HSORB/4X,4HNOD
     1E,3X, 3HAVG, 9X,
     1     1H1,9X,1H2,9X,1H3,9X,1H4
     2         /6H AXIAL/5H NODE)
  203 FORMAT ( I5,4X,12(F6.4,4X))
      END
```

```
@ ELT PRDESB,1,710719, 62348    , 1

      SUBROUTINE PRDESB(IBED)
C
C
       COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,       PK (2,20),PCO2I  ,TS  (20)     *NEW
      1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),     *NEW
      2TC2 (20),W (4,20),PT (20),           GMR ,GMW,GVIS, PN2,PO2,            *NEW
      3              ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),         *NEW
      4AVX(20),RHOG(20),RHOS3(20),RHOS(20),RHOC(20),RHOX(20),                  *NEW
      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                       *NEW
      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),             *NEW
      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                   *NEW
      8                               HXG(20),HXS(20),HXC(20),HSG(20),         *NEW
      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,        *NEW
      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                      *NEW
      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,               *NEW
      1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),      *NEW
      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),        *NEW
      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),         *NEW
      3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3     *NEW
      4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),      *NEW
      5            WM(2),TIME,CYCLE,DTO,   DTMAX,WI,TI,PCO2C,                  *NEW
      6VOLCAB,RCO2C,                                                           *NEW
      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS           *NEW
       DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,               *NEW
      1      CP1,CP2,X,   C1P,C2P,C3P,D1P                                      *NEW
       DIMENSION AVLD(41)                                                      **-1
       EQUIVALENCE(NDX,NDX1)
C
       AVMSLD=0.0
       AVSGLD=0.0
       AVRCO2=0.0
       AVRH2O=0.0
       TIMEM=60.*TIME
       WRITE(6,499)IBED
       WRITE(6,100) NCYCLE,TIME ,TIMEM,DT
       WRITE (6,101)
       WRITE (6,102)(N,PT(N),TG(N),TS(N),TC(N),TX(N),N=1,NDX)
       IF(( NPSET(1) .GT. 0) .OR. (NPSET(2) .GT. 0)) GO TO 99
    99 WRITE (6,202)
       N1=NDXM+1
       NDR3=NDR4-1
       DO 20 N= 1, NDXM
       SUMMS=0.0
       SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
       IF(NDR4 .EQ. 2) AVLD(N) = SUMMS
       IF(NDR4.EQ.2) GO TO 20
       DO 22 NR=2,NDR3
    22 SUMMS=SUMMS+W(NR,N)
       AVLD(N)=SUMMS/NDR3
    20 CONTINUE
       DO 30 N= N1,NDX1
       SUMMS=0.0
       SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
       IF(NDR4.EQ.2) AVLD(N) = SUMMS
       IF(NDR4.EQ.2) GO TO 30
       DO 33 NR=2, NDR3
    33 SUMMS=SUMMS+W(NR,N)
       AVLD(N)=SUMMS/NDR3
```

```
   30 CONTINUE
      IF(NDXMAC .EQ. 0) GO TO 35
      SUM=0.
      DO 31 N= 1, NDXMAC
   31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVMSLD = SUM/WTACMS
   35 CONTINUE
      IF((NDX1-NDXM) .EQ. 0) GO TO 40
      SUM=0.
      DO 32 N= N1,NDX1
   32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
      AVSGLD=SUM/WTSG
   40 CONTINUE
      DO 10 N=1,NDX
   10 WRITE (6,203)N, AVLD(N)
     1                   ,(W(NR,N),NR=1,NDR4)
      IF(TIME .LT. 1.1E-5) AVMSL1=AVMSLD
      IF(TIME .LT. 1.1E-5) AVSGL1=AVSGLD
      AVRCO2=WTACMS*(AVMSL1-AVMSLD)/TIME
      AVRH2O=WTSG*(AVSGL1-AVSGLD)/TIME
      DIMENSION F1(9),F2(9),F3(9),F4(9),  F5(9),F6(9),F7(9),F8(9),F9(9)
      WRITE(6,205) F1,AVMSLD,F2,AVSGLD,F3,AVRCO2,F4,AVRH2O,F5,TOTKWH,
     1F6,TOTHTC,           F8,PCO2A, F9,VCO2A
  205 FORMAT(////(9A6,F8.4,6X,9A6,F8.4 ))
      DATA F1/' AVG CO2 LOADING IN CO2 SORBENT (LB/LB)'/
      DATA F2/' AVG H2O LOADING IN DESICCANT (LB/LB)'/
      DATA F3/' TIME AVG CO2 DESORPTION RATE (LB/HR)'/
      DATA F4/' TIME AVG H2O DESORPTION RATE (LB/HR)'/
      DATA F5/' ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)'/
      DATA F6/' HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)'/
      DATA F7/' CABIN CO2 PARTIAL PRESSURE (MM)'/
      DATA F8/' ACCUMULATOR CO2 PRESSURE (PSIA)'/
      DATA F9/' CO2 ACCUMULATOR VOLUME (CU FT)'/
C
  499 FORMAT(8H1BED NO.  I3)
  100 FORMAT (1H0,16HDESORPTION CYCLE  I3/
     1           3X,5HTIME=,F9.5,1X2HHR,F12.3,1X,3HMIN,
     1                                     5X,15HTIME INCREMENT=F7.5,1X2HHR)
  101 FORMAT (//2X,10HAXIAL NODE,10X,14HTOTAL PRESS,MM,6X,14HGAS TEMP,DE
     1G F,5X,19HSORBENT TEMP, DEG F,2X,18HCOOLANT TEMP,DEG F,3X,19HHX CO
     2RE TEMP, DEG F  )
  102 FORMAT(/(I9,11X,5(F14.4,6X)))
  103 FORMAT (/21H0CO2 DESORPTION RATE=F7.4,1X5HLB/HR,5X,20HH2O DESORPTI
     1ON RATE=F7.4,1X5HLB/HR)
  200 FORMAT (1H0/2X,10HAXIAL NODE,13X,9HMOLE FRAC,7X,
     12X,13HCO2 RATE,M/HR,6X,13HH2O RATE,M/HR)
  201 FORMAT(/(I9,11X,3(4X,F12.6,4X)))
  202 FORMAT (//  31H0LOADING AT INTERIOR OF SORBENT//4X,4HSORB/4X,4HNOD
     1E,3X, 3HAVG, 9X,
     1     1H1,9X,1H2,9X,1H3,9X,1H4
     2        /6H AXIAL/5H NODE)
  203 FORMAT ( I5,4X,12(F6.4,4X))
      RETURN
      END
```


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@ ELT READ1,1,710712, 56801 , 1

```
      SUBROUTINE READ1
      COMMON/B1/
     1                ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
     2AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
     3CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
     4POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
     5            NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20)
      COMMON/B1A/
     1                                  HXG(20),HXS(20),HXC(20),HSG(20),
     2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,
     3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
     1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
      NAMELIST/DB  / ABED,AVC,    ASX,AGX,     AVX,RHOG,RHOSB,RHOS,RHOC,
     1RHOX,CPG, CPC,CPX,CPP,DX,NPSET,NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,
     2POUT,TIMET,              PUMP,VPUMP,IDSORB,CPL,DP
      NAMELIST/DBA  / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,    TCIN,HTR1,TMAX
     1,WCC
      EQUIVALENCE(TCIN,T268)
      READ (5,DB)
      WRITE(6,DB)
      READ(5,DBA)
      WRITE(6,DBA)
      DO 10 N=1,NDX1
   10 ASG(N)=6.*RHOSB(N)/RHOS(N)/DP(N)
      RETURN
      END
```

@ ELT READ2,1,710712, 56801 , 1

```
      SUBROUTINE READ2
      COMMON/B1D/
     1                                  HXG(20),HXS(20),HXC(20),HSG(20),
     2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,
     3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
     1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
      NAMELIST/DBD  / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,    TCIN,HTR1,TMAX
     1,WCC
      EQUIVALENCE(TCIN,T268)
      READ(5,DBD)
      WRITE(6,DBD)
      RETURN
      END
```

@ ELT READ3,1,710712, 56802 , 1

```
      SUBROUTINE READ3
      COMMON/B2/
     1                ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
     2AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
     3CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
     4POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
     5            NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20)
      COMMON/B2A/
     1                                  HXG(20),HXS(20),HXC(20),HSG(20),
     2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,
     3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
     1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
      NAMELIST/MB  / ABED,AVC,    ASX,AGX,     AVX,RHOG,RHOSB,RHOS,RHOC,
     1RHOX,CPG, CPC,CPX,CPP,DX,NPSET,NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,
     2POUT,TIMET,              PUMP,VPUMP,IDSORB,CPL,DP
      NAMELIST/MBA  / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,    TCIN,HTR1,TMAX
     1,WCC
      EQUIVALENCE(TCIN,T268)
      DATA RHOG/ 20*0.0003/
      READ(5,MB)
      WRITE(6,MB)
      READ(5,MBA)
      WRITE(6,MBA)
      DO 10 N=1,NDX1
   10 ASG(N)=6.*RHOSB(N)/RHOS(N)/DP(N)
      RETURN
      END
```


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```
@ ELT READ4,1,710712, 56803    , 1
      SUBROUTINE READ4
      COMMON/B2D/
     1                                                    HXG(20),HXS(20),HXC(20),HSG(20),
     2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,
     3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
     1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
      NAMELIST/MBD  / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,    TCIN,HTR1,TMAX
     1,WCC
      EQUIVALENCE(TCIN,T268)
      READ(5,MBD)
      WRITE(6,MBD)
      RETURN
      END
```

```
@ ELT START,1,710719, 62350     , 1

      SUBROUTINE START
C
      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)    *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),     *NEW
     2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,PO2,           *NEW
     3              ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),       *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                     *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),           *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                 *NEW
     8                            HXG(20),HXS(20),HXC(20),HSG(20),          *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,      *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                    *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,             *NEW
     1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),     *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),       *NEW
     3FR(2,20),       P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3   *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),    *NEW
     5               WM(2),TIME,CYCLE,DTO,   DTMAX,WI,TI,PCO2C,             *NEW
     6VOLCAB,RCO2C,                                                         *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS         *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,             *NEW
     1        CP1,CP2,X,   C1P,C2P,C3P,D1P                                  *NEW
C                                                                           **-1
      DO 5 N=1,NDX1
      I=IFN(N,NDXM)
      CPS(N)=CPP(N)+W(1,N)*CPL(I)
    5 RS(N)=DP(N)/2.000
      DO 30 N= 1, NDX1
   30 VOIDF(N) = 1. - RHOSB(N)/RHOS(N)
      DO 115 N=1,NDX1
  115 A(N)= GMR/ABED(N)/PA/GMW
      NDR=NDR4-1
      NDR2= 2*NDR
      NDR3=NDR2+1
      DO 10 I=1,NDX1
      VS(I)=4./3.*3.1416*RS(I)**3
      DVS(I)=VS(I)/NDR
      DVS1(I)=DVS(I)/2
      RS1(I,1)=0.
      DO 10 K=2,NDR3
   10 RS1(I,K)=CBRT(3./4./3.1416*(4./3.*3.1416*RS1(I,K-1)**3+DVS1(I)))
      DO 11 I=1,NDX1
      CR1(I,1)=DVS1(I)*RHOS(I)
      CR2(I,1)=0.
      CR3(I,1)=4.*3.1416*RS1(I,2)**2*DIF(I)/(RS1(I,3)-RS1(I,1))*RHOS(I)
      DO 11 K=2,NDR4
      CR1(I,K)=DVS(I)*RHOS(I)
      CR2(I,K)=4.*3.1416*RS1(I,2*K-2)**2*DIF(I)/(RS1(I,2*K-1)-RS1(I,2*K-
     13))*RHOS(I)
   11 CR3(I,K)=4.*3.1416*RS1(I,2*K)**2*DIF(I)/(RS1(I,2*K+1)-RS1(I,2*K-1)
     1)*RHOS(I)
      DO 12 N=1,NDX1
   12 CR1(N,NDR4)=CR1(N,1)
      RETURN
      END
```

@ ELT TGLCOL,1,710514, 58260 , 1

```
      SUBROUTINE TGLCOL(TC,NDXMAX,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
     1AVC, NOGLIN,DTO,TS1,TS2,TX1,TX2,TC1,TC2)
      DIMENSION C1(20),C2(20),C3(20),D(20),TC(1),TX(1),HXC(1),AVC(1),
     1          TS1(1),TS2(1),TX1(1),TX2(1),TC1(1),TC2(1)
      DIMENSION UC(1),RHOC(1),CPC(1),AXC(1)
      DN=DT+DTO
      DO 10 N=1,NDXMAX
      CC1=-UC(N)
      CC2=HXC(N)/(CPC(N)*RHOC(N))*AVC(N)*0.5
      IF( UC(N) .GT. 0.) GO TO 5
      C3(N)=-CC1/DX
      C2(N)=1./DN+CC2-C3(N)
      C1(N)=0.0
      GO TO 10
    5 C1(N) = CC1/DX
      C2(N) = 1./DN + CC2 - C1(N)
      C3(N) = 0.0
   10 D(N)=TC2(N)/DN+CC2*TX1(N)*2. - CC2*TC2(N)
      C1(NOGLIN) = 0.
      C3(NOGLIN) = 0.
      D(NOGLIN)=D(NOGLIN) +ABS(UC(NOGLIN))/DX*T268
      CALL FDEQIM(C1,C2,C3,D,TC,NDXMAX)
      RETURN
      END
```

@ ELT TSORB,1,710719, 62351 , 1

```
      SUBROUTINE TSORB
      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)    *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),     *NEW
     2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,PO2,           *NEW
     3               ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),      *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                     *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),           *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                 *NEW
     8                                HXG(20),HXS(20),HXC(20),HSG(20),      *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,      *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                    *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,             *NEW
     1RS1(20,9),       A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),    *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),       *NEW
     3FR(2,20),        P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3  *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),    *NEW
     5             WM(2),TIME,CYCLE,DTO,    DTMAX,WI,TI,PCO2C,              *NEW
     6VOLCAB,RCO2C,                                                         *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS         *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,             *NEW
     1         CP1,CP2,X,   C1P,C2P,C3P,D1P                                 *NEW
      DIMENSION S1(41),S2(41),S3(41),B1(41)                                 **-1
      DO 10 N=1,NDX1
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=CS1(N)*(1.0+T1)
      CS2(N)=CS2(N)*(1.0+T1)
      B1(N) =TS2(N)+CS1(N)*PT(N)-CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)-WS(N))+
     1P3(N)*PT(N))+T*(ASG(N)*HSG(N)*TG (N)+ASX(N)*HXS(N)*
     2                                                TX1(N))-T1*TS2(N)
      S1(N)=-T*SK(N)/DX/DX
      S2(N)=1.-2.*S1(N)+T1
      S3(N)=S1(N)
   10 CONTINUE
      S2(1)=S2(1)+S1(1)
      S1(1)=0.0
      S2(NDX1)=S2(NDX1)+S3(NDX1)
      S3(NDX1)=0.
      NSG=NDXM+1
      S2(NDXM)=S2(NDXM)+S3(NDXM)
      S3(NDXM)=0.
      S2(NSG)= S2(NSG)+S1(NSG)
      S1(NSG)=0.0
      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1)
      RETURN
      END
```

```
@ ELT TSORBA,1,710719, 62352    , 1
      SUBROUTINE TSORBA
      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,      PK (2,20),PCO2I  ,TS  (20)        *NEW
     1,TC  (20),TX  (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),         *NEW
     2TC2 (20),W (4,20),PT (20),            GMR ,GMW,GVIS, PN2,PO2,             *NEW
     3                  ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),       *NEW
     4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),                    *NEW
     5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),                         *NEW
     6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),               *NEW
     7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),                     *NEW
     8                                     HXG(20),HXS(20),HXC(20),HSG(20),     *NEW
     9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,          *NEW
     1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,                                        *NEW
     1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A,                 *NEW
     1RS1(20,9),         A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),      *NEW
     1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),          *NEW
     2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),           *NEW
     3FR(2,20),        P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3      *NEW
     4(20,4),  C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),        *NEW
     5              WM(2),TIME,CYCLE,DTO,    DTMAX,WI,TI,PCO2C,                 *NEW
     6VOLCAB,RCO2C,                                                             *NEW
     7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS             *NEW
      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,                 *NEW
     1       CP1,CP2,X,    C1P,C2P,C3P,D1P                                      *NEW
      DIMENSION S1(41),S2(41),S3(41),B1(41)                                     **-1
      DO 10 N=1,NDX1
      T=(DT+DTO)/CPS(N)/RHOSB(N)
      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
      CS1(N)=CS1(N)*(1.0+T1)
      CS2(N)=CS2(N)*(1.0+T1)
      I=IFN(N,NDXM)
      TGAVG1=TG(N)
      B1(N) =TS2(N)*CS1(N)*
     1PK(I,N)
     2                          -CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)-WS(N))+
     1P3(N)*
     2PK(I,N)
     3               )+T*(ASG(N)*HSG(N)*TGAVG1+
     4ASX(N)*HXS(N)*TX1(N))-T1*TS2(N)
      S1(N)=-T*SK(N)/DX/DX
      S2(N)=1.-2.*S1(N)+T1
      S3(N)=S1(N)
   10 CONTINUE
      S2(1)=S2(1)+S1(1)
      S1(1)=0.0
      S2(NDX1)=S2(NDX1)+S3(NDX1)
      S3(NDX1)=0.
      NSG=NDXM+1
      S2(NDXM)=S2(NDXM)+S3(NDXM)
      S3(NDXM)=0.
      S2(NSG)= S2(NSG)+S1(NSG)
      S1(NSG)=0.0
      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1)
      RETURN
      END
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@ ELT XYZMAP,1,710514, 38520   , 1
          FUNCTION XYZMAP(IND,X,Y,NP,Z,NC,IDX,IDY,BX,BY,ANS)
      C
      C   FUNCTION XYZMAP HAS THE CAPABILITY OF SUBROUTINES MAPRDY + LAGIN2.
      C   ANSWER IS ALSO AVAILABLE AT LOCATION (ANS).
      C   ALSO CAPABLE OF HANDLING MAP THAT HAS Z-LINES CROSSING EACH OTHER.
      C
      C   X=ABSISSA, Y=ORDINATE, Z=THIRD PARAMETER.
      C
      C   IND=0, Z=F(X,Y), (EQUIVALENT TO SUBROUTINE MAPRDY).
      C   IND=1, Y=F(X,Z), (EQUIVALENT TO SUBROUTINE MAPRDY).
      C   IND=-1, Y=F(X) ONLY, (EQUIVALENT TO LAGIN2), THEN Z,NC,IDY, AND AY
      C    ARE DUMMY VARIABLES THAT ARE NOT NEEDED IN ACTUAL INTERPOLATION.
      C
      C   XS MUST BE STORED IN ASCENDING ORDER FOR EACH Z.  SIMILARLY,
      C   SMALLEST Z BE FED IN AS Z(1), ZS ARE IN ASCENDING ORDER.
      C   XS NEED NOT BE THE SAME VALUES FOR VARIOUS ZS.
      C   X,Y AND Z ARE TO BE DIMENSIONED IN THE MAIN (OR CALLING) PROGRAM,
      C   THEY MUST BE DIMENSIONED NOT LESS THAN *** X(NP*NC), Y(NP*NC) AND
      C    Z(NC) *** NOTE NC MAY NOT BE GREATER THAN 20 ***
      C
      C   NP=NUMBER OF POINTS PER CURVE (OR NUMBER OF X,Y PAIRS FOR EACH Z).
      C   NC=NUMBER OF CURVES (OR NUMBER OF ZS), 1 TO A MAXIMUM OF 20
      C
      C   IDX=POINTS USED FOR INTERPOLATION IN X-DIRECTION,
      C   IDY=POINTS USED FOR INTERPOLATION IN Y-DIRECTION (IND=0),
      C                                     OR IN Z-DIRECTION (IND=1).
      C   IDX OR  IDY CAN EITHER BE 2 OR 3 ONLY.
      C   BX=FIRST INDEPENDENT VARIABLE.
      C   BY=SECOND INDEPENDENT VARIABLE, (WHEN IND=0 OR 1 ONLY).
      C   BY=Y INDEPENDENT VARIABLE, WHEN (IND=0).
      C   BY=Z INDEPENDENT VARIABLE, WHEN (IND=1).
      C   ANS=DEPENDENT VARIABLE Z(X=AX,Y=AY), WHEN IND=0,
      C   ANS=DEPENDENT VARIABLE Y(X=AX,Z=AY), WHEN IND=1,
      C   ANS=DEPENDENT VARIABLE Y(X=AX),  WHEN IND=-1.
      C
      C   NO PRINT OUT, IF DATA OFF THE RANGE OF MAP OR CURVE.
      C   THEN, USE 2-POINT INTERPOLATIONS AUTOMATICALLY,
      C
      C   ******************************************************************
      C   XS, YS, AND ZS ARE READ IN IN MAIN PROGRAM RECOMMENDED AS FOLLOWS,
      C4100 FORMAT(8I10)                                               *****
      C4101 FORMAT(8F10.0)                                             *****
      C   ********** FOR IND=0 OR 1 ****************************************
      C4101 READ (5,4100)         NP,NC                                *****
      C     DO 100 N=1,NC                                              *****
      C     READ (5,4101)         Z(N)                                 *****
      C     ME=N*NP                                                    *****
      C     MS=ME-NP+1                                                 *****
      C 100 READ (5,4101)          (X(M),Y(M),M=MS,ME)                 *****
      C   ********** FOR IND=-1 ********************************************
      C     READ (5,4100)          NP                             **********
      C     READ (5,4101)         (X(M),Y(M),M=1,NP)              **********
      C   ******************************************************************
      C
          DIMENSION X(2),Y(2),Z(2),ZZ(20),ZX(20)
          JS=1
          IF (IND) 105,106,103
      103 DO 104 I=1,NC
```

```
 104 ZX(I)=Z(I)
     GO TO 141
 105 JE=1
     GO TO 108
 106 DO 107 I=1,NC
 107 ZZ(I)=Z(I)
     JE=NC
     NCROSS=0
 108 DO 126 J=JS,JE
     JX2=(J-1)*NP
     DO 109 I=1,NP
     J2=I+JX2
     IF (BX-X(J2)) 114,110,109
 109 CONTINUE
     GO TO 119
 110 ANS=Y(J2)
     GO TO 123
 114 IF(I-IDX)120,120,119
 119 JX2=J2-IDX
 120 IS=JX2+1
     IE=JX2+IDX
     IF(IDX.GT.2) GO TO 122
 121 ANS=(Y(IE)*(BX-X(IS))-Y(IS)*(BX-X(IE)))/(X(IE)-X(IS))
     GO TO 123
 122 IM=IS+1
     G1=(BX-X(IS))/(X(IM)-X(IE))
     G2=(BX-X(IM))/(X(IE)-X(IS))
     G3=(BX-X(IE))/(X(IS)-X(IM))
     ANS=-Y(IS)*G2*G3-G1*(Y(IM)*G3+Y(IE)*G2)
 123 IF (IND) 158,125,124
 124 ZZ(J)=ANS
     GO TO 126
 125 ZX(J)=ANS
     IF(ANS.LT.ZX(1)) NCROSS=1
 126 CONTINUE
     IF(IND.NE.0) GO TO 1151
     IF(NCROSS.EQ.0) GO TO 141
C
     DO 130 K=2,NC
     JMIN=K-1
     DO 129 IP=K,NC
     IF (ZX(IP)-ZX(JMIN)) 128,128,129
 128 JMIN=IP
 129 CONTINUE
     IK=K-1
     C1=ZX(JMIN)
     Z1=ZZ(JMIN)
     ZX(JMIN)=ZX(IK)
     ZZ(JMIN)=ZZ(IK)
     ZX(IK)=C1
 130 ZZ(IK)=Z1
C
 141 ICPY= IDY-1
     DO 142 I=1,NC
     IF(BY-ZX(I))145,144,142
 142 CONTINUE
     JS=NC-ICPY
     GO TO 147
 144 JS=I
     IF (IND.EQ.0) GO TO 151
```

```
      JE=JS
      GO TO 108
  145 IF(I.LE.IDY) GO TO 147
  146 JS=I-ICPY
  147 JE=JS+ICPY
      IF (IND) 108,1152,108
C     Y=F(X,Z) OR Z=F(X,Y) CALCULATION DEPENDING ON IND=0 OR 1.
  151 ANS=ZZ(JS)
      GO TO 158
 1151 IF(JE.EQ.JS) GO TO 151
 1152 IF(IDY.GT.2) GO TO 153
  152 ANS=(ZZ(JE)*(BY-ZX(JS))-ZZ(JS)*(BY-ZX(JE)))/(ZX(JE)-ZX(JS))
      GO TO 158
  153 JM=JS+1
      G1=(BY-ZX(JS))/(ZX(JM)-ZX(JE))
      G2=(BY-ZX(JM))/(ZX(JE)-ZX(JS))
      G3=(BY-ZX(JE))/(ZX(JS)-ZX(JM))
      ANS=-ZZ(JS)*G2*G3-G1*(ZZ(JM)*G3+ZZ(JE)*G2)
  158 XYZMAP=ANS
      RETURN
      END
```


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