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**A TRANSIENT PERFORMANCE METHOD
FOR CO₂ REMOVAL WITH
REGENERABLE ADSORBENTS**

**CASE FILE
COPY**

72-8786

October 1972

Prepared Under
Contract No. NAS 1-8559

by

AIRESEARCH MANUFACTURING COMPANY
Los Angeles, California

for

National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia

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Prepared by
K.C. Hwang

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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 CO₂ or water removal, and composite beds of two sorbents for simultaneous humidity control and CO₂ 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 CO₂-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 CO₂-removal bed is taken into account in predicting the CO₂ 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 H₂O-save/CO₂-dump, and
- 4-bed H₂O-CO₂-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

<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
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)
AVH2QP		Average poisoning rate of molecular sieves by H ₂ O, (lb-H ₂ O)/hr
AVMSLD		Average CO ₂ -loading of all active molecular sieve sorbents, lb-CO ₂ /(lb-molecular sieves)
AVPH2O		Average outlet P _{H₂O} , mm Hg
AVRCO2		Average CO ₂ adsorption or desorption rate, lb-CO ₂ /hr
AVRH2O		Average H ₂ O adsorption or desorption rate, lb-H ₂ O/hr
AVSGLD		Average H ₂ O-loading of desiccant sorbents, lb-H ₂ O/(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)



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>	
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	}	Coefficients in equation	
CP2			$PC3 \cdot \left(P_{ks,t+\Delta t} - X_k P_{t+\Delta t} \right) = CP1 + CP2 \cdot P_{t+\Delta t}$
CR1	}	Coefficients in following equation which is merely another form of Equation (2-28).	
CR2			$CR1 \cdot \frac{W_{k,M,(t+\Delta t)} - W_{k,M,t}}{(\Delta t)} = CR2 \cdot (W_{k,(M-1),(t+\Delta t)} - W_{k,M,(t+\Delta t)} + CR3 \cdot (W_{k,M,(t+\Delta t)} - W_{k,(M+1),(t+\Delta t)})$
CR3			
CS1	}	Coefficients in equation	
CS2			$T_{s,(t+\Delta t)} - T_{s,t} = DS + CS1 \cdot P_{(t+\Delta t)} - CS2 \cdot P_{ks,(t+\Delta t)}$
CYCLE		Cycle time per one adsorption or one desorption half-cycle, hr	
C1	}	Coefficients in equation	
C2			$C1 \cdot W_{(t+\Delta t),(M-1)} + C2 \cdot W_{(t+\Delta t),M} + C3 \cdot W_{(t+\Delta t),(M+1)} = DI$
C3			
CIP	}	Coefficients in equation	
C2P			$CIP \cdot P_{(t+\Delta t),(N-1)} + C2P \cdot P_{(t+\Delta t),N} + C3P \cdot P_{(t+\Delta t),(N+1)} = DIP$
C3P			
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	



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
DPC ϕ 2C		Cabin CO ₂ partial pressure increase in one time increment, mm Hg
DS		See CSI
DT ϕ		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 ₂ O, during desorption, FR(1,N) is CO ₂ rate, FR(2,N) is H ₂ O 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)(°F)(hr)



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
HGS,HSG	h_{sg}	Heat transfer coefficient between sorbent and gas, based on a_{sg} , Btu/(sq ft)(°F)(hr)
HSX,HXS	h_{xs}	Effective heat transfer coefficient between heat exchanger primary plate and sorbent, Btu/(sq ft)(°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



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
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 ≠ 0, heat balances will be performed
PA	P	System total pressure during adsorption, mm Hg
PC ϕ 2C		CO ₂ partial pressure in cabin, mm Hg
PC ϕ 2I		CO ₂ partial pressure at adsorption bed inlet, mm Hg
PC1		$\left. \begin{aligned} & \text{Coefficients in equation for desorption pressure} \\ & \frac{P(t+\Delta t), N - P(t, N)}{(\Delta t)} = PC1 \cdot \frac{P(t+\Delta t), (N-1) - 2P(t+\Delta t), N + P(t+\Delta t), (N+1)}{(\Delta x)^2} \\ & + PC2 \cdot \frac{P(t+\Delta t), (N+1) - P(t+\Delta t), (N-1)}{2(\Delta x)} \\ & + PC3 \cdot [P_{ks}(t+\Delta t) - X_k P(t+\Delta t)] \end{aligned} \right\}$
PC2		
PC3		
PH ϕ I		Inlet H ₂ O partial pressure, mm Hg
PK	P _k	P · X _k ; partial pressure of component k in bulk gas stream, mm Hg
P ϕ UT		10 tabulated desorption outlet pressures at TIMET, mm Hg
PT	P	Total pressure in bulk gas stream, mm Hg
P1		$\left. \begin{aligned} & \text{Coefficients in equation} \\ & P_{ks}(t+\Delta t) = P1 + P2 \cdot (W_{k,s}(t+\Delta t) - W_{k,s,t}) + P3 \cdot P \end{aligned} \right\}$
P2		
P3		
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



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
	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) (°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) (°F/ft)
SUMPTM		Quantity $\int_{t=zero}^t P_{H_2O, outlet} \cdot (\Delta t)$, (mm) (hr)
TC	T_c	Coolant temperature, °F
TC1		Coolant temperature at time, $t-\Delta t$
TC2		Coolant temperature at time, $t-2\Delta t$
TG	T_g	Gas temperature, °F
TGI	T_{gi}	Inlet gas temperature for adsorption cycle, °F



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
TI		Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}\text{F}$
TIME	t	Time from beginning of each adsorption or desorption period, hr
TIMEM		Time above in minutes.
TIMET		10 times at which POUT are tabulated, hr
TKX	k_x	Thermal conductivity of heat exchanger core metal, Btu/(hr) (sq ft) ($^{\circ}\text{F}/\text{ft}$)
TOTC02		Total amount of CO_2 adsorbed since beginning of adsorption period, lb
TOTH02		Total amount of H_2O adsorbed since beginning of adsorption period, lb
TS	T_s	Sorbent temperature, $^{\circ}\text{F}$
TS1		Sorbent temperature at time $t - (\Delta t)$, $^{\circ}\text{F}$
TS2		Sorbent temperature at time $t - 2(\Delta t)$, $^{\circ}\text{F}$
TX	T_x	Heat exchanger core metal temperature, $^{\circ}\text{F}$
TX1		Heat exchanger core metal temperature at time $t - (\Delta t)$, $^{\circ}\text{F}$
TX2		Heat exchanger core metal temperature at time $t - 2(\Delta t)$, $^{\circ}\text{F}$
T268	T_{268}	Inlet glycol temperature, $^{\circ}\text{F}$
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



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
VØIDF	f	Void fraction of bed
VØLCAB		Cabin volume for atmosphere, cu ft; use VOLCAB = 10 ²⁰ , for constant PC02C
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 ₂ O 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 CO₂ 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 CO₂-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.

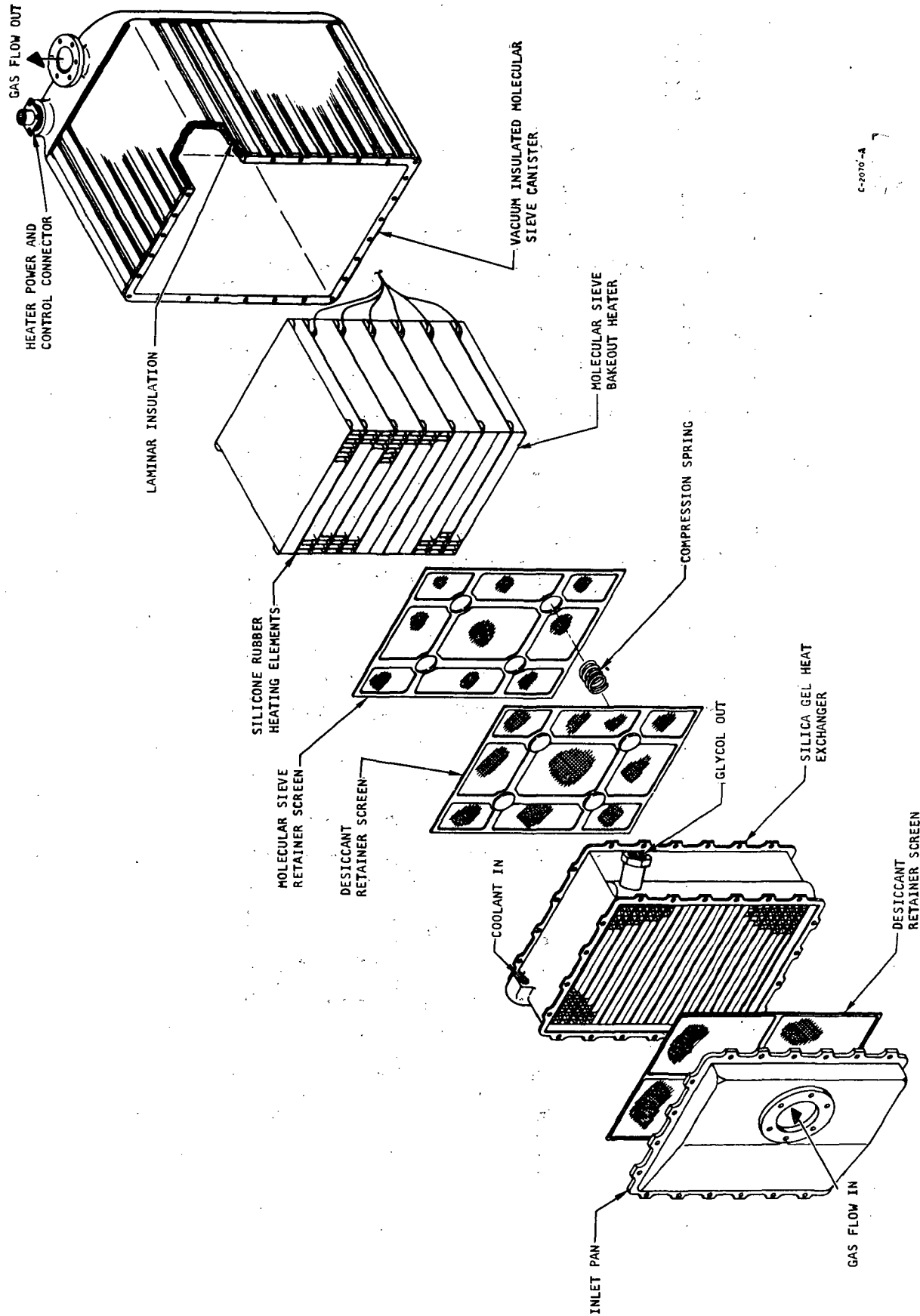
PROGRAM CAPABILITIES

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 CO₂ 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



C-2070-A

Figure 1-1. Typical Adsorbent Canister



S-50350

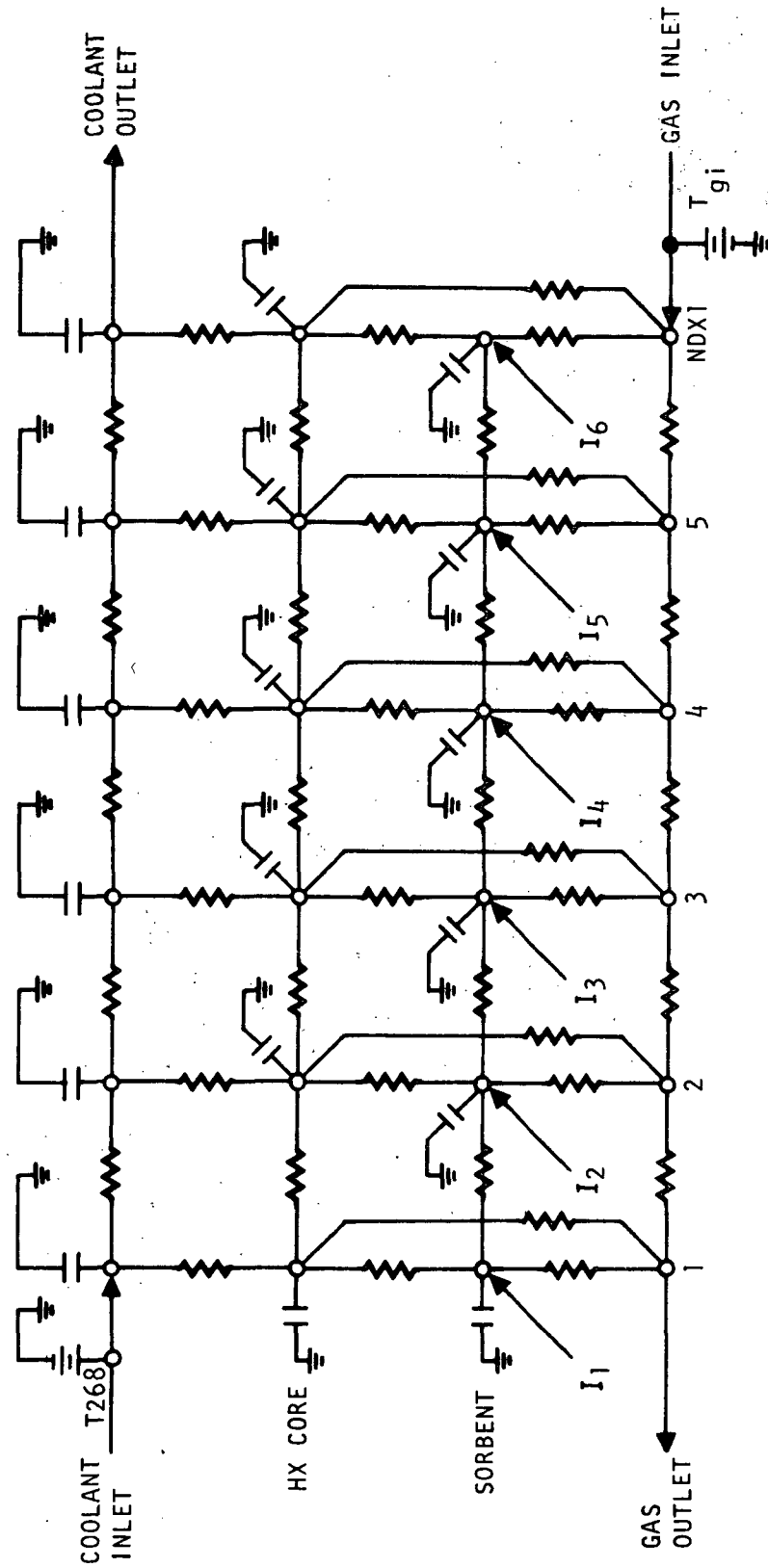
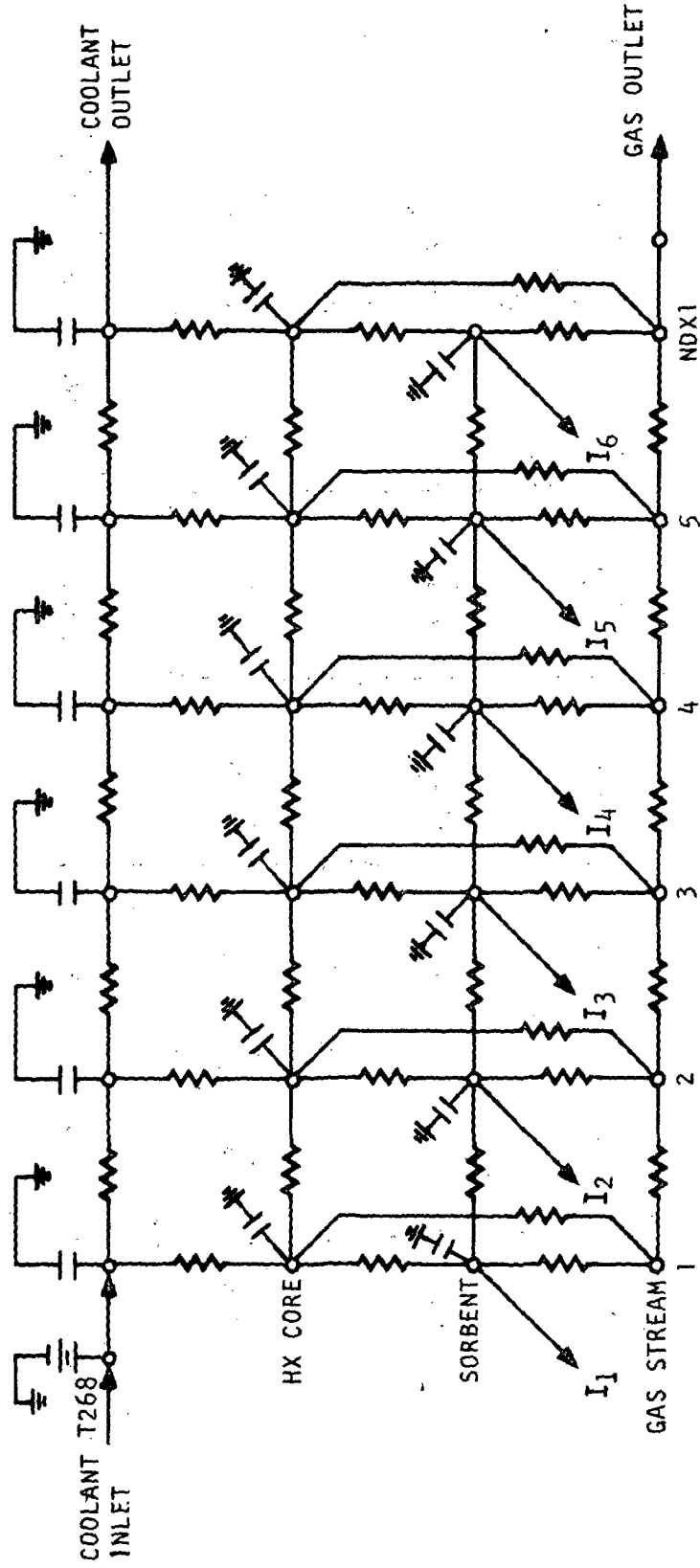
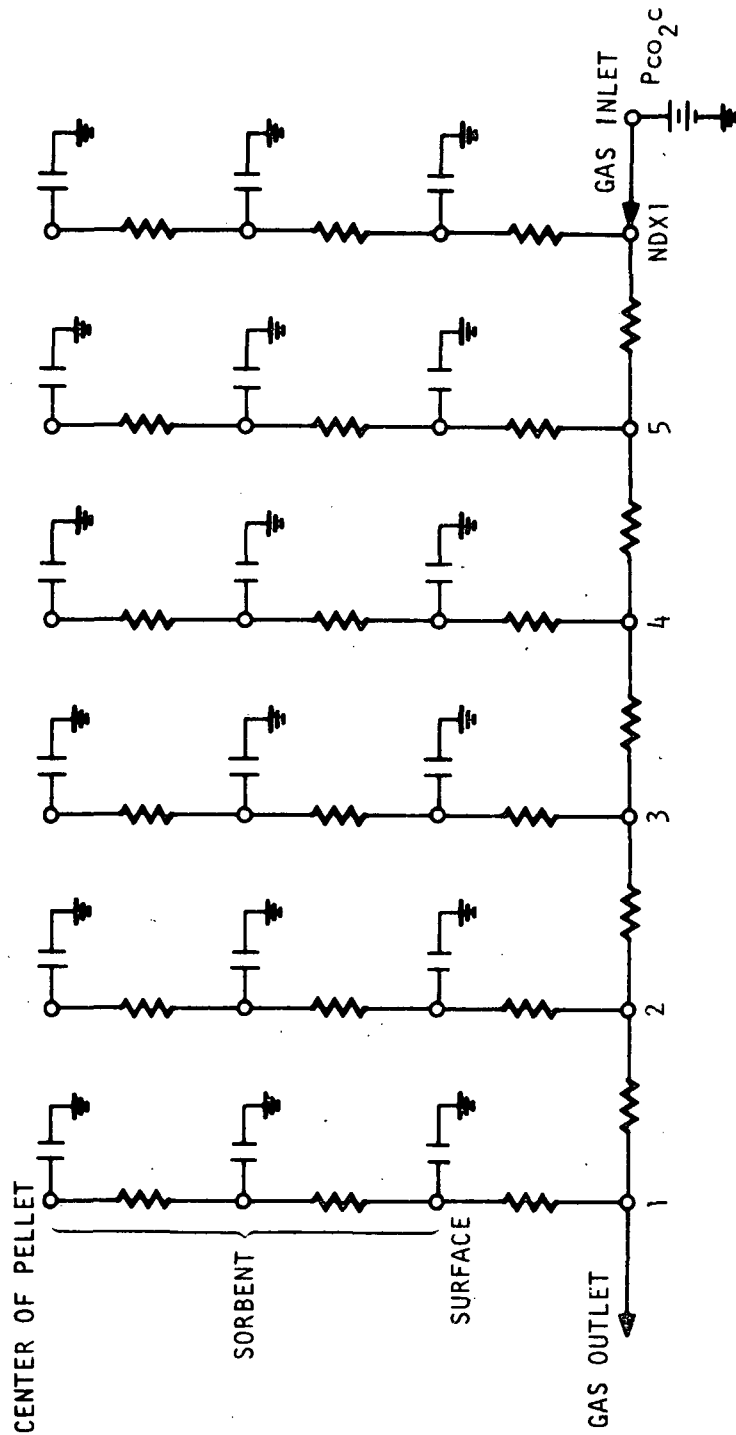


Figure 1-2. Thermal Network for Sorbent Bed During Adsorption



S-50353

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



S-50351

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

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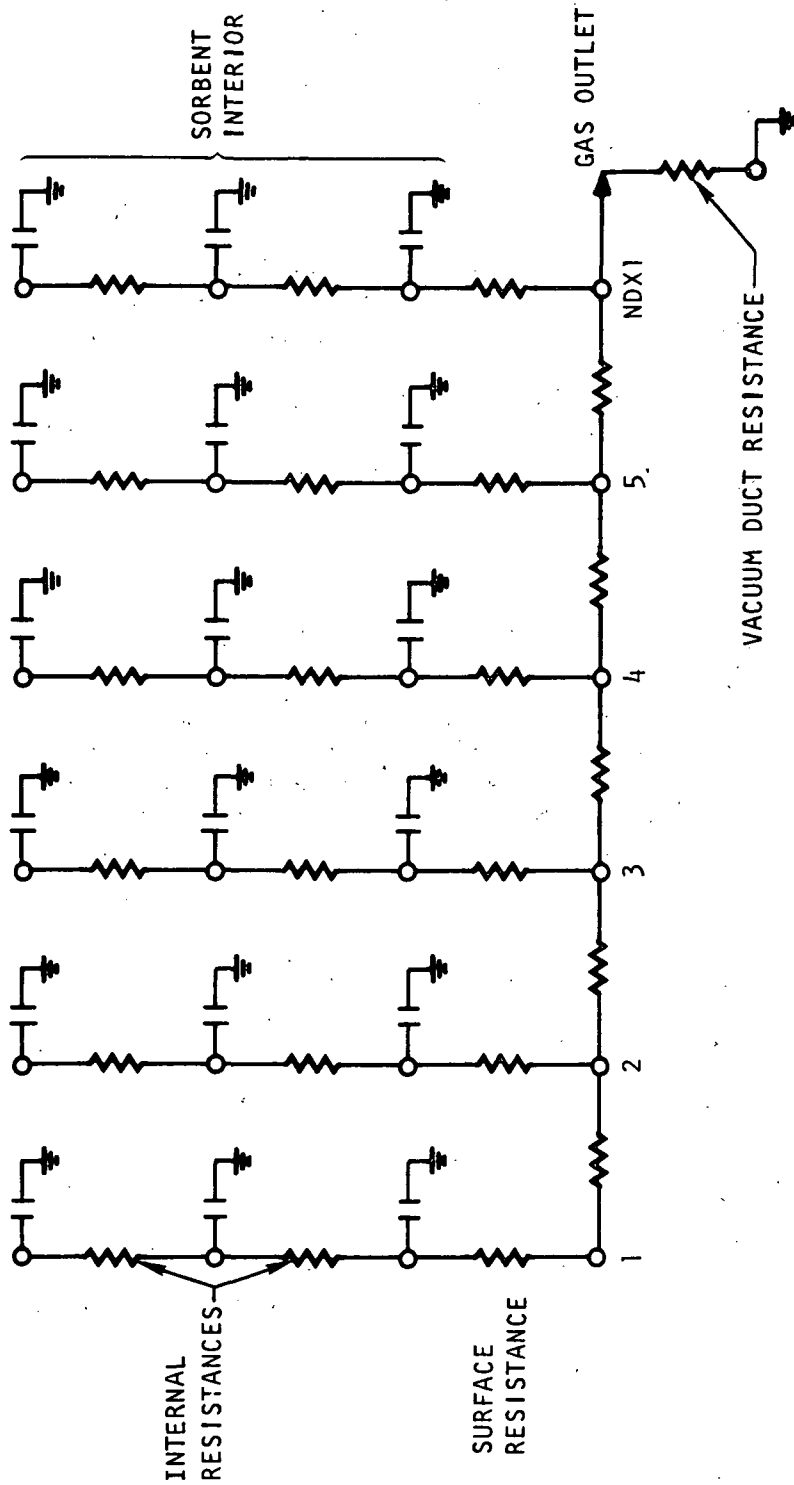


Figure 1-5. Mass Transfer Model for Sorbent Bed During Vacuum Desorption

specified performance requirements, if operating parameters are given. To optimize an entire vacuum-dump CO₂-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 H₂O over the desiccant and CO₂ 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 CO₂ and H₂O 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.

<u>Assumption</u>	<u>Description</u>
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

$$\frac{\partial w_k}{\partial t} = \frac{D_k}{\rho_s} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial w_k}{\partial r} \right) \quad (2-1)$$



Boundary conditions are

$$\frac{\partial w_k}{\partial r} = 0 \text{ at } r = 0 \quad (2-2)$$

$$-\rho_s D_k \frac{\partial w_k}{\partial r} = M_k K_g (p_{k_s} - P \cdot X_k) \text{ at } r = r_s \quad (2-3)$$

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,

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

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

$$T_g = T_{gi} \text{ at } x = x_0 \text{ (i.e., process gas inlet)} \quad (2-5)$$

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

$$T_g = T_s \text{ at } x = 0 \quad (2-6)$$

Energy Equation for Sorbent

$$\begin{aligned} \frac{\partial T_s}{\partial t} = & \frac{\partial}{\partial x} \left(k_s A \frac{\partial T_s}{\partial x} \right) + \left(\frac{a_{sg} \cdot h_{sg}}{C_{ps} \cdot \rho_{sb}} \right) (T_g - T_s) + \left(\frac{a_{xs} \cdot h_{xs}}{C_{ps} \cdot \rho_{sb}} \right) (T_x - T_s) \\ & + \left(\frac{a_{sg} \cdot K_g}{C_{ps} \cdot \rho_{sb}} \right) (p_k - p_{ks}) \cdot (\Delta H_k) \end{aligned} \quad (2-7)$$

This equation is subject to the conditions

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

$$\frac{\partial T_s}{\partial x} = 0 \text{ at } x = x_0 \quad (2-8)$$

Energy Equation for Coolant Stream

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

The boundary condition for this equation is

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

Energy Equation for Heat Exchanger Core Metal

$$\begin{aligned} (c_{px} \cdot \rho_x) \frac{\partial T_x}{\partial t} = \frac{\partial}{\partial x} \left(k_x \frac{\partial T_x}{\partial x} \right) + a_{vx} \cdot \left[h_{xs} (T_s - T_x) \right. \\ \left. + h_{xg} (T_g - T_x) + h_{xc} (T_c - T_x) \right] \end{aligned} \quad (2-11)$$

Boundary conditions for this equation are

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

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.

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

This has an inlet condition

$$P_k = P_{k, \text{inlet}} \text{ at } x = x_o \quad (2-14)$$

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

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

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

and u_g is related to pressure gradient by

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

Also, by differentiating the perfect gas law

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

one obtains

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

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:

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

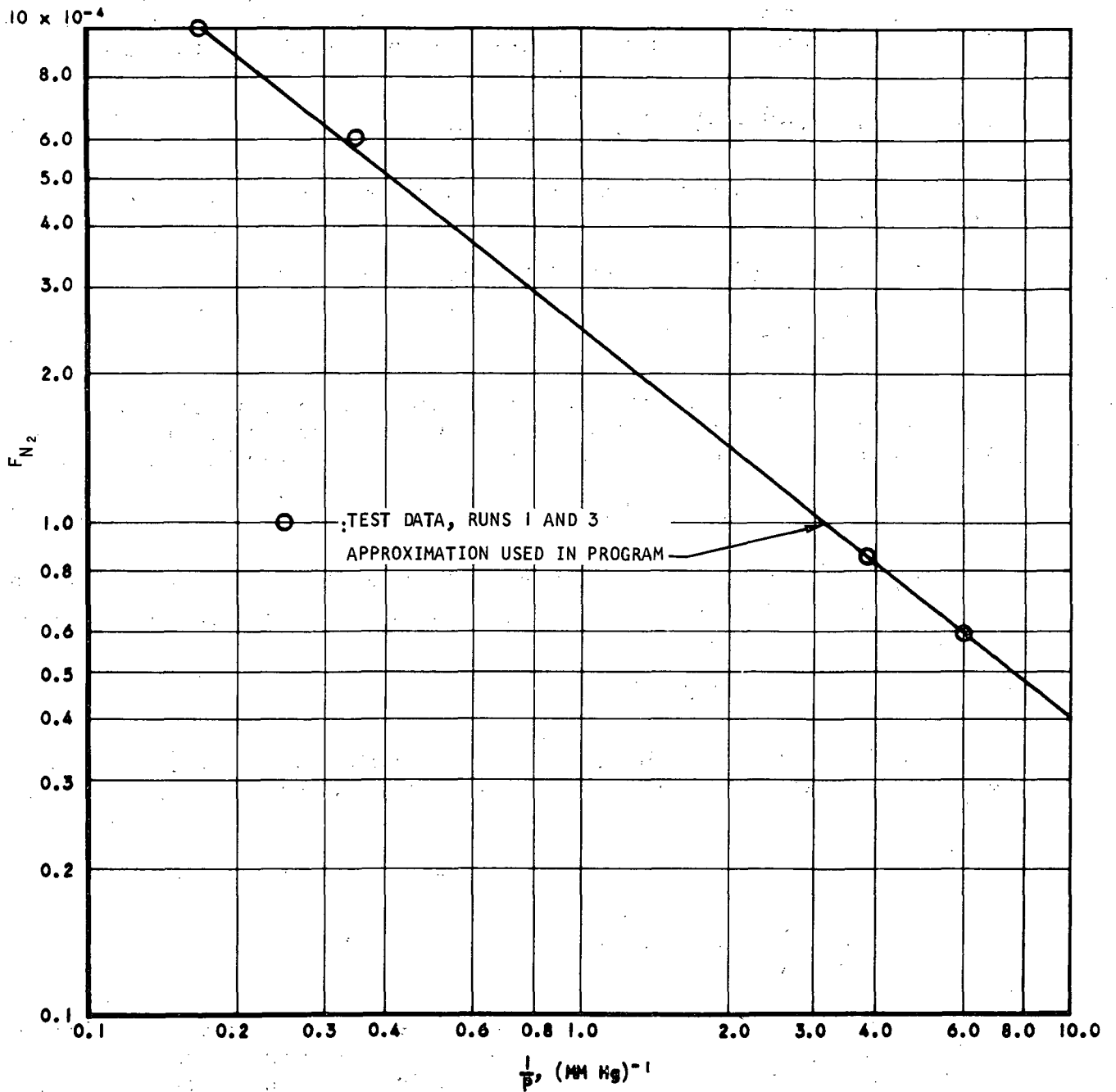
Equation (2-20) is used in the program for calculating pressure changes during the desorption half cycle.

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

$$\frac{F_{N_2} G \cdot R \cdot T_g}{M_g} = \frac{(P_1^2 - P_2^2)}{2 (x_2 - x_1)} \quad (2-21)$$

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





A-24666

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



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

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.

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

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

$$\frac{\partial P}{\partial x} = 0 \text{ at } x = 0 \quad (2-24)$$

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

$$f \cdot \rho_g \cdot u_g \cdot A = W_D(P) \quad (2-25)$$

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.

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

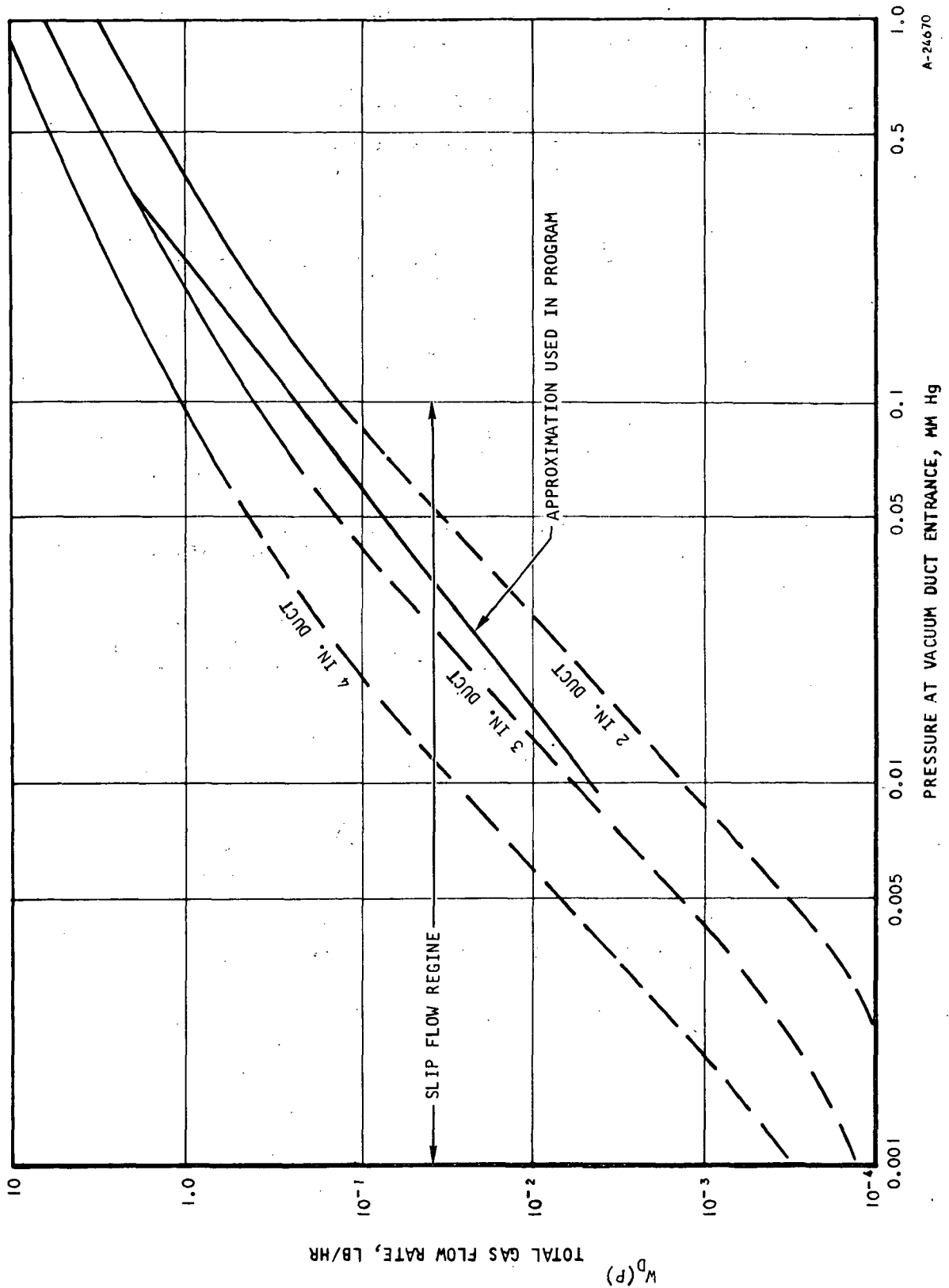
The dotted lines in Figure 2-2 were the estimated flow rates for 18 in. long ducts. The resistance contributed by the gas valve were not included in these calculations.

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

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

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.





A-24670

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

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

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

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

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

and

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

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

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



Energy Equation for Gas Stream

Equation (2-4) is approximated by

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

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.

$$\begin{aligned} \frac{T_{s(t+\Delta t),N} - T_{s(t-\Delta t),N}}{2 \cdot (\Delta t)} &= \frac{l}{c_{ps} \cdot \rho_{sb} \cdot (\Delta x)^2 A_N} \cdot \left[k_{s(N+1/2)} \cdot A_{(N+1/2)} \cdot (T_{s(t+\Delta t),(N+1)} - T_{s(t+\Delta t),N}) - k_{s(N-1/2)} \cdot A_{(N-1/2)} \cdot (T_{s(t+\Delta t),N} - T_{s(t+\Delta t),(N-1)}) \right] \\ &+ \left(\frac{a_{sg} \cdot h_{sg}}{c_{ps} \cdot \rho_{sb}} \right)_N \cdot T_{g,t,N} \\ &- \left[\frac{T_{s(t+\Delta t),N} + T_{s(t-\Delta t),N}}{2} \right] + \left(\frac{a_{xs} \cdot h_{xs}}{c_{ps} \cdot \rho_{sb}} \right)_N \left[T_{x,t,N} - \frac{T_{s(t+\Delta t),N} + T_{s(t-\Delta t),N}}{2} \right] \\ &+ \left(\frac{a_{sg} \cdot K_g}{c_{ps} \cdot \rho_{sb}} \right)_N \\ &\cdot \left[p_{k(t+\Delta t),N} - p_{ks(t+\Delta t),N} \right] \cdot (\Delta H_k) \end{aligned} \quad (2-32)$$



Energy Equation for Coolant Stream

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

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

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

Energy Equation for Heat-Exchanger Core Metal

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

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

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

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

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

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

Adsorption Material Balance for K-th Component in Gas Stream

Equation (2-13) is approximated by

$$\frac{P_{k(N-1)} - P_{k(N)}}{(\Delta x)} = \left(\frac{P \cdot M_g}{f \cdot \rho_g \cdot u_g} \right) \cdot a_{sg} \cdot k_g \cdot (P_{ks(N-1)} - P_{k(N-1)}) \quad (2-35)$$



Pressure Equations for Desorption

Equation (2-20) is represented by

$$\begin{aligned} \frac{P_{(t+\Delta t),N} - P_{t,N}}{(\Delta t)} &= \frac{P_{t,N}}{F_{t,N} \cdot (\Delta x)^2} \left[P_{(t+\Delta t),(N-1)} - 2P_{(t+\Delta t),N} \right. \\ &+ \left. P_{(t+\Delta t),(N+1)} \right] + \left(\frac{P}{f \cdot C \cdot A} \right)_{t,N} \cdot \frac{1}{2(\Delta x)^2} \\ &\left[\left(\frac{A \cdot f \cdot C}{F} \right)_{t,N} - \left(\frac{A \cdot f \cdot C}{F} \right)_{t,(N-1)} \right] \cdot \left[P_{(t+\Delta t),(N+1)} - P_{(t+\Delta t),(N-1)} \right] \\ &+ \left(\frac{P}{C \cdot f} \right)_{t,N} \cdot a_{sg} \cdot K_g \cdot \left[P_{ks(t+\Delta t),N} - P_{(t+\Delta t),N} \cdot X_{k,t,N} \right] \end{aligned} \quad (2-36)$$

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

$$-\frac{P_{(NDX1+1)} - P_{NDX1}}{F \cdot (\Delta x)} = \left(\frac{11.2 P^{0.715}}{f \cdot \rho_g \cdot A} \right)_{NDX1} P_{NDX1} \quad (2-37)$$

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)

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

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

$$C_{1,NDX1} Y_{(NDX1-1),(t+\Delta t)} + C_{2,NDX1} Y_{(NDX1),(t+\Delta t)} = D_{NDX1} \quad (2-40)$$

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

$$B_1 = \frac{C_{3,1}}{C_{2,1}} \quad (2-41)$$

$$B_N = \frac{C_{3N}}{(C_{2N} - C_{1N} B_{N-1})} \quad (N = 2, 3, \dots, NDX1) \quad (2-42)$$

$$Q_1 = \frac{D_1}{C_{2_1}} \quad (2-43)$$

$$Q_N = \frac{(D_N - C_{1N} Q_{N-1})}{(B_N - C_{1N} B_{N-1})}, \quad (N = 2, 3, \dots, NDX1) \quad (2-44)$$

$$Y_{NDX1} = Q_{NDX1} \quad (2-45)$$

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

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

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

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

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

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

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:

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

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

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

where

$$P_1 = \left[P_{k,s,t} + D_s \left(\frac{\partial p_k^*}{\partial T_s} \right) \right] / \left[1 + C_{s2} \left(\frac{\partial p_k^*}{\partial T_s} \right) \right] \quad (2-51)$$

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

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

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:

$$\begin{aligned} \frac{P_{N,(t+\Delta t)} - P_{N,(t)}}{(\Delta t)} &= P_{C1} \cdot \frac{P_{(N-1),(t+\Delta t)}^{-2} \cdot P_{N,(t+\Delta t)} + P_{(N+1),(t+\Delta t)}}{(\Delta x)^2} \\ &+ P_{C2} \cdot \frac{P_{(N+1),(t+\Delta t)} - P_{(N-1),(t+\Delta t)}}{2 \cdot (\Delta x)} \\ &+ P_{C3} \cdot [P_{ks} - X_k \cdot P_{N,(t+\Delta t)}] \end{aligned} \quad (2-54)$$

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

$$P_{C3} \cdot [P_{ks} - X_k \cdot P_{N,(t+\Delta t)}] = C_{P1N} + C_{P2N} \cdot P_{N,(t+\Delta t)} \quad (2-55)$$

where
$$C_{P1,N} = P_{C3,N} \cdot \left[P_{1,N} + P_{2,N} \cdot \left\{ Q_{s,N} - W_{k_s}(t) \right\} \right] \quad (2-56)$$

$$C_{P2,N} = P_{C3,N} \cdot \left[P_{2,N} \cdot D_{2,N} + P_{3,N} \right] - X_k \quad (2-57)$$

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

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

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

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

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

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

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:

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

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

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



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

$$- \left[\frac{C_{P2,N}}{\left(\frac{f \cdot \rho_g \cdot u_g}{P \cdot M_g} \right)} \right]$$

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

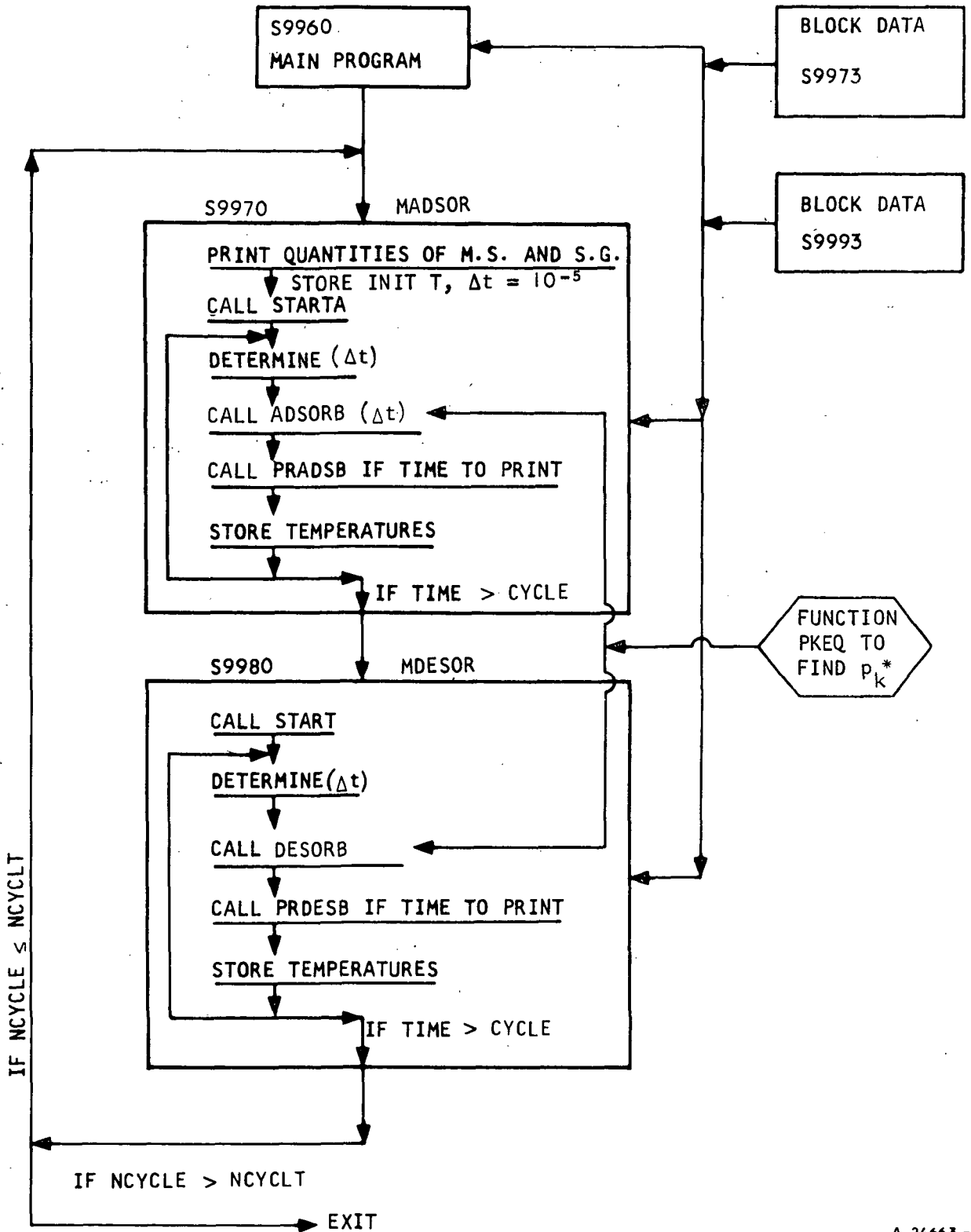
$$C_{P2,N} = a_{sg} \cdot K_g \cdot (P_2 \cdot D_2 + P_3 - 1) \quad (2-69)$$

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.





A-24663 -A

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

<u>FORTRAN</u> <u>Symbol</u>	<u>Maximum</u> <u>Dimension</u>	<u>Definition</u>
		<u>Bed Configuration</u>
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 molecular 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



<u>FORTRAN Symbol</u>	<u>Maximum Dimension</u>	<u>Definition</u>
<u>Sorbent Properties</u>		
ASG	(41)	Sorbent specific surface area, sq ft/(cu ft of bed)
CPS	(41)	Sorbent specific heat, Btu/(lb) ($^{\circ}$ 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) ($^{\circ}$ F/ft)
<u>Coolant Properties</u>		
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) ($^{\circ}$ F)
NOG		Node to which coolant is added
RHOC	(41)	Coolant density, lb/(cu ft)
T268		Coolant inlet temperature, $^{\circ}$ F
UC	(41)	Coolant velocity, ft/hr
<u>Heat Transfer Coefficients</u>		
HSG	(41)	Heat transfer coefficient, sorbent to gas, Btu/(hr) (sq ft)($^{\circ}$ F)
HXC	(41)	Heat transfer coefficient, heat exchanger to coolant Btu/(sq ft) (hr)($^{\circ}$ F)
HXG	(41)	Heat transfer coefficient, heat exchanger to process gas, Btu/(sq ft) ($^{\circ}$ F) (hr)
HXS	(41)	Heat transfer coefficient, heat exchanger to sorbent, Btu/(sq ft)(hr)($^{\circ}$ F)



<u>FORTRAN Symbol</u>	<u>Maximum Dimension</u>	<u>Definition</u>
<u>Initial Conditions</u>		
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)
<u>Mass Transfer Properties</u>		
DIF	(41)	Internal diffusivity, sq ft/hr
GK	(41)	External surface mass transfer coefficient, lb-mole/(hr)(sq ft)(mm Hg)
<u>Process Gas Stream Properties</u>		
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 ₂ O)
<u>HX Core Properties</u>		
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)



<u>FORTRAN</u> <u>Symbol</u>	<u>Maximum</u> <u>Dimension</u>	<u>Definition</u>
<u>Miscellaneous Control Parameters</u>		
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
NDTC ϕ N		If NDTC ϕ N = 1, Δt will be selected such that $\Delta T = TI$, $\Delta W = WI$ for time step; if NDTC ϕ N = 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 \neq 0, nonisothermal analysis
TI		Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}F$
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 NDTC ϕ N need to appear only once either in S9973 or S9993.



Input Variables Required by S9973 Only

<u>FORTTRAN</u> <u>Symbol</u>	<u>Definition</u>
GMR	Process gas flow rate, lb/hr
GMW	Process gas molecular weight
PA	System total pressure, mm Hg
PC ϕ 2C	Initial CO ₂ partial pressure in cabin, mm Hg
PH2 ϕ 1	Inlet H ₂ O partial pressure, mm Hg
TGI	Inlet process gas temperature, °F
V ϕ LCAB	Cabin volume for atmosphere, cu ft; use V ϕ LCAB = 10 ²⁰ , for constant PC ϕ 2C
RC ϕ 2C	Rate of CO ₂ generation in cabin, lb CO ₂ per hr

Input Variables Required by S9993 Only

<u>FORTTRAN</u> <u>Symbol</u>	<u>Definition</u>
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 (10)	10 pairs of exit pressure vs time data to be used
TIMET (10)	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 CO₂ pressure over the molecular sieve sorbent at a loading of W lb CO₂/lb sieve and at T °F; and for ID = 2, computes H₂O vapor pressure over the desiccant sorbent at a loading of W lb H₂O/lb desiccant and T °F.



Equilibrium isotherms can be used in tabular forms and p_k^* 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 to 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 CO₂ 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 CO₂-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 CO₂ 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 CO₂ 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 CoefficientsI. 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

$\frac{\text{Btu}}{\text{hr ft}^2 \text{ } ^\circ\text{F}}$ and an effective particle diameter of:

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



MOLECULAR SIEVE CANISTER COMPUTER NODAL STRUCTURE

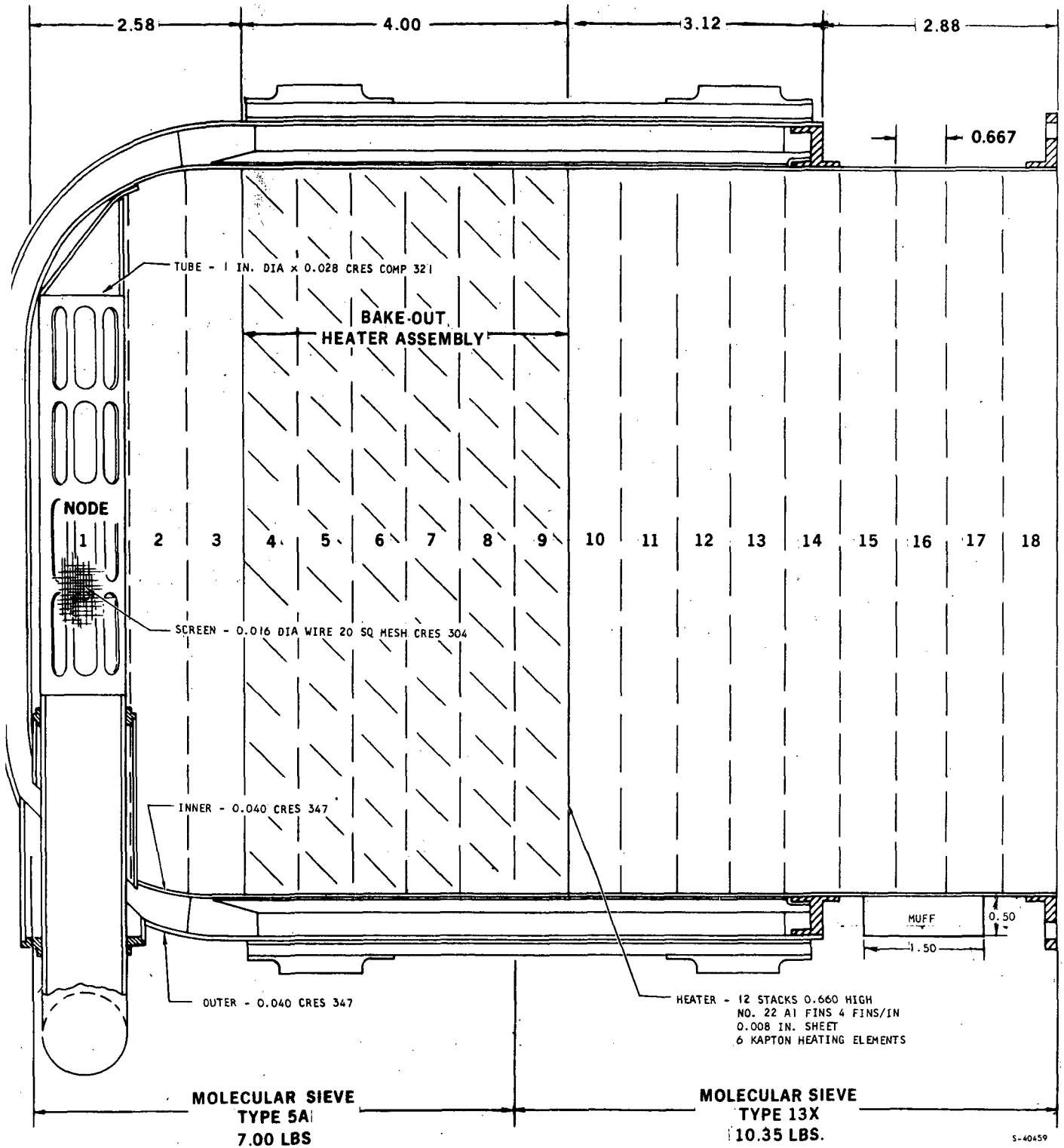


Figure 4-1. Molecular Sieve Canister for Airlock Application



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

During desorption, the thermal conductivity of the gas drops to 0.0022 Btu/hr ft °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:

$$\left. \begin{array}{l} SK = 0.10 \text{ Btu/(sq ft)(hr)(}^\circ\text{F/ft)} \\ \text{and for desorption,} \\ SK = 0.08 \text{ Btu/(sq ft)(hr)(}^\circ\text{F/ft)} \end{array} \right\} \text{bulk pack}$$

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

$$\left. \begin{array}{l} SK = 11.6 \\ \text{and during desorption,} \\ SK = 11.6 \end{array} \right\} \text{heat exchanger}$$

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.

$$\text{HXG} = 0.01475/0.146 = 0.101$$

during desorption

$$\text{HXG} = 0.0022/0.146 = 0.0151$$

Diffusion Coefficients for CO₂ in 5A and H₂O 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

$$\text{GK}_{\text{CO}_2} - 5\text{A} = 0.9 \times 10^{-4}$$

$$\text{GK}_{\text{H}_2\text{O}} - 13\text{X} = 5.0 \times 10^{-3}$$

2. Desorption

$$\text{GK}_{\text{CO}_2} - 5\text{A} = 5.0 \times 10^{-4}$$

$$\text{GK}_{\text{H}_2\text{O}} - 13\text{X} = 1.0 \times 10^{-3}$$

Properties of Sorbents

1. Sorbent Density

$$\text{RH}\emptyset\text{S} = 64 \text{ lb/cu ft}$$

2. Bulk Density

$$\text{RH}\emptyset\text{SB} = 45 \text{ lb/cu ft in bulk pack}$$

$$\text{RH}\emptyset\text{SB} = 36 \text{ lb/cu ft in heater core}$$



Heat of Adsorption

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

$$DH = 400 \text{ for } CO_2 \text{ on } 5A \text{ (Btu/lb)}$$

$$DH = 1400 \text{ for } H_2O \text{ on } 13X \text{ (Btu/lb)}$$

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:

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

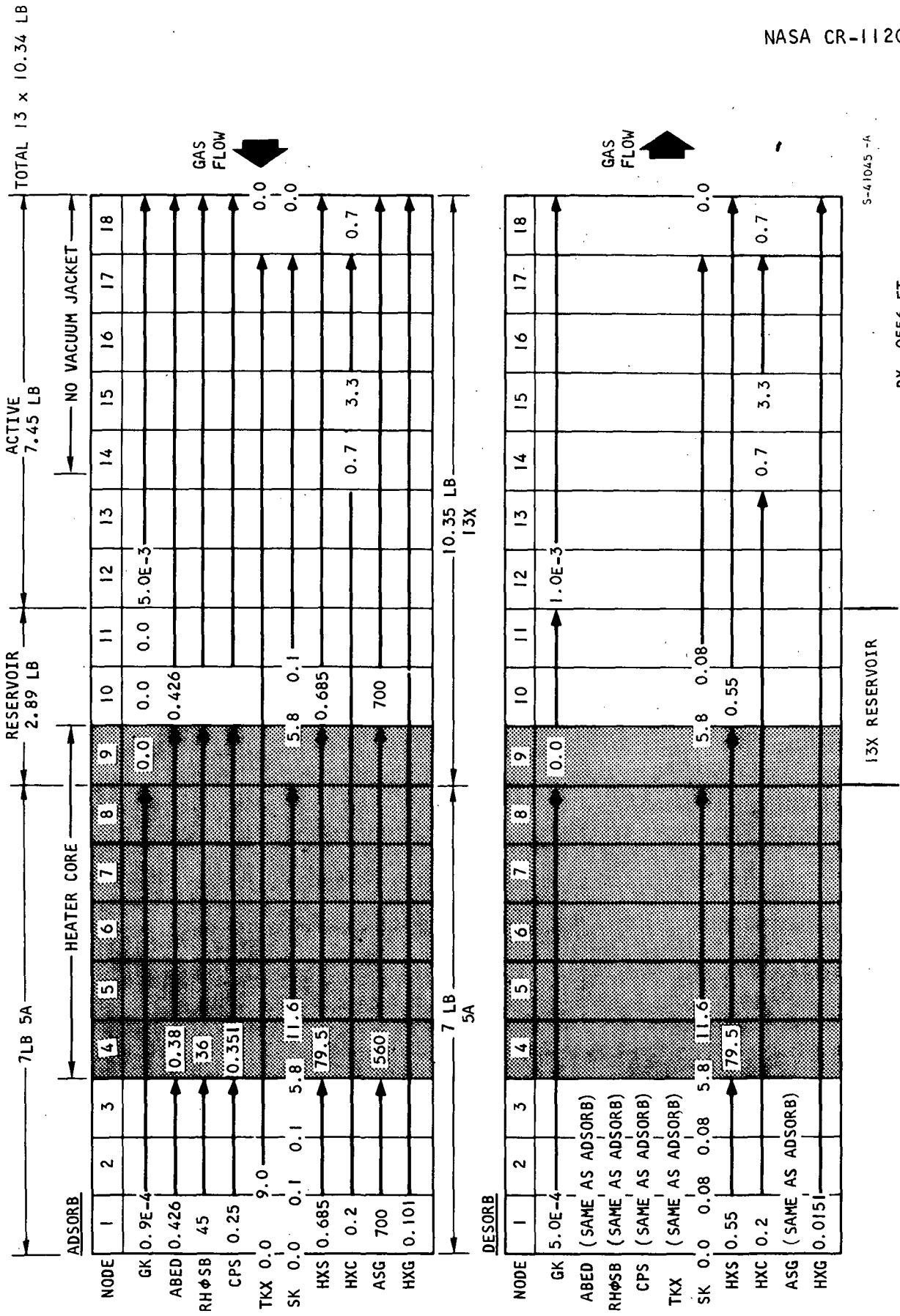
This equation is used in subroutine DESORB for the present simulation.

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.



S-41045 -A

DX=.0556 FT

Figure 4-2. Computer Nodal Parameters For Air-Lock CO₂ Removal System

INPUT DATA FOR EXAMPLE PROBLEM



e ELT 59973.1.690617, 53904 .1

```

000001      BLOCK DATA
000002      C INPUT DATA TO ADSORB
000003      COMMON /BLOK2/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000004      1HXG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS1(2), R
000005      2S1(2,41), RHOS(2), UG(41), WH(2), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000006      3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000007      41), PC3(41), ASG(41), ASX(41), AGX(41), CJP(41), C2B(41), C3B(41), D1P(41)
000008      5, FRI(2,41), RS(2), NOX1, NDR4, DA, DT, GK(41), OH(41), SK(41), PI(41), P2(41)
000009      6, P3(41), WS(41), CRI(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000010      7(21,41), CP1(41), CP2(41), X(41), VOIDF(41), TIME
000011      8, AXI(41), RHOCI(41), CPC(41), T268, AVX(41), TRX(41), CPX(41), RHOX(41)
000012      9, NOG, PK(2,41), PCO21, PH2O1, GMR, GMW, TGI, PA, PY(41), CPS(41), HSG(41)
000013      COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
000014      DOUBLE PRECISION W
000015      COMMON /BLOK6/ NCYCLT
000016      COMMON/BLOK10/ NPRINT,DTMAX,NDTCON
000017      COMMON /BLOK12/ NTEMP
000018      COMMON /BLOK13/ W1, T1
000019      COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RCO2C
000020      COMMON /BLOK17/ NSTART
000021      DIMENSION AXSI(41), AXG(41), AGS(41), HSX(41), HGX(41), HGS(41), ACX(41),
000022      1HCX(41)
000023      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
000024      1,HGS),(AXC,ACX),(HXC,HCX)
000025
000026      C BED CONFIGURATION
000027
000028      DATA ABED/3*.426,6*.38,9*.426,23*0./
000029      DATA NDX1, NDXM, NDXMAC, NDR4, DX / 18, 11, 8, 2, 0, 0, 556/
000030      DATA AGX / 41*6.18/
000031      DATA ASX... / 41*6.18/
000032      C SORBENT PROPERTIES
000033
000034      DATA ASG/3*780.,6*560.,9*700.,23*0.0/
000035      DATA CPS/3*.25,6*.351,9*.25,23*0.0/
000036      DATA RHOS /64., 64., /
000037      DATA RHOSB/3*45.,6*36.,9*45.,23*0.0/
000038      DATA SK/0.2*1.5,8.5*11.6,5.8*1.23*0.0/
000039      C COOLANT PROPERTIES
000040
000041      DATA AVC / 41*100, /
000042      DATA CPC/41*1.E20/
000043      DATA NOG / 1 /
000044      DATA T268 /70./
000045      DATA UC/41*0.0/
000046      C HEAT TRANSFER COEFFICIENTS
000047
000048      DATA HSG / 41*20, /
000049      DATA HXC/13*0.2,7,3*3.3,7,23*0.0/
000050      DATA HXG/18*0.101,23*0.0/
000051      DATA HXS/3*.685,6*79,5,9*.685,23*0.0/
000052      C INITIAL CONDITIONS
000053
000054      DATA TC/14*70.,3*65.,24*70.0/
000055      DATA TG/8*55.,3*75.,3*80.,75.,60.,40.,23,23*50./
000056      DATA TS/8*55.,3*75.,3*80.,75.,60.,40.,23,23*50./
000057      DATA TX/41*70./
000058

```



```

000059 DATA X/168*.03100.63*1.0-3.721*.1200.21*.13700.21*.1500.21*.1600.
000060 121*.1800.21*.200.21*.20500.483*1.0-3/
000061 C MASS TRANSFER PROPERTIES
000062 C
000063 DATA DIF/41*4.E-4/
000064 DATA GK /R*0.9E-4, 3*0.0, 7*5.E-3, 23*0.0 /
000065 C PROCESS GAS STREAM PROPERTIES
000066 C
000067 DATA CPG /41*0.23 /
000068 DATA DH / 11*400., 7*1400., 23*0.0 /
000069 DATA WM / 44.0, 18.0 /
000070 C HX CORE PROPERTIES
000071 DATA AVX /41*375./
000072 DATA CPX / 41*0.11/
000073 DATA RHDX/ 41*490./
000074 DATA TKX / 0., 17*9.0, 23*0.0/
000075 C MISCELLANEOUS CONTROL PARAMETERS
000076 C
000077 DATA CYCLE/ 0.25/
000078 DATA NTEMP/ 1/
000079 DATA NCYCLI, NSTART/10.10/
000080 DATA NPRINT/10/
000081 DATA W1,T1/ 0.005, 1.5 /
000082 DATA DTMAX/ 0.005 /
000083 DATA NDTCOM/ 1 /
000084 C ADSORB PARAMETERS
000085 C
000086 DATA PC02C, PH201, TGI /7.0, 10., 52. /
000087 DATA VOLCAB, RC02C / 320.01, 0.281 /
000088 DATA GMR, GMW/10., 28.04/
000089 DATA PA/258./
000090 END

```



0 ELT S9993,1,690617, 53905 .1

```

000001      BLOCK DATA
000002      C INPUT DATA TO DESORB
000003      COMMON /BLOK1/ ABEDI(41), A(41), AVC(41), CPG(41), RHOG(41),
000004      1HXG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS(2), R
000005      2S1(2,41), RHOS(2), UC(41), WM(2), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000006      3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000007      41), PC3(41), ASS(41), ASX(41), AGX(41), CIP(41), C2P(41), C3P(41), DIP(41)
000008      5, FR(2,41), RS(2), NDX1, NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
000009      6, P3(41), WS(41), CRI(2,21), CR3(2,21), CR3(2,21), C3(21,41), B(21,41),
000010      7(21,41), CP1(41), CP2(41), X(41), VOIDF(41), TIME
000011      8, AXCI(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41)
000012      9, NOG, PK(2,41), PCO21, PH201, GMR, GMW, TGI, PA, PT(41), CPS(41), HSG(41)
000013      DOUBLE PRECISION CIP, C2P, C3P, DIP
000014      DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, P1, P2, P3, C3, Q, B,
000015      1. CP1, CP2, X, DT
000016      COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
000017      DOUBLE PRECISION W
000018      COMMON /BLOK4/ POUT(10), TIMET(10), NBCOUT, NPSET(3)
000019      COMMON /BLOK6/ NCYCLT
000020      COMMON /BLOK10/ NPRINT, DTHAX, NDTCON
000021      COMMON /BLOK12/ NTEMP
000022      COMMON /BLOK13/ WI, TI
000023      COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RCO2C
000024      COMMON /BLOK17/ NSTART
000025      DIMENSION AXS(41), AXG(41), AGS(41), HXS(41), HGS(41), ACX(41),
000026      1HXC(41)
000027      EQUIVALENCE (ASX, AXS), (ACX, AXG), (ASG, AGS), (HXS, HXS), (HXC, HXC), (HSG
000028      1, HGS), (AXG, ACX), (HXC, HXC)
000029      C BED CONFIGURATION
000030
000031      DATA ABEDI/3, 426, 68, 38, 9, 424, 2380, /
000032      DATA NDX1, NDXM, NDXMAC, NDR4, DX / 18, 11, 8, 2, 0, 0556/
000033      DATA AGX / 41, 6, 18/
000034      DATA ASX / 41, 6, 18/
000035      C SORBENT PROPERTIES
000036
000037      DATA ASG/3, 700, 6, 540, 9, 700, 2380, 0, /
000038      DATA CPS/3, 25, 6, 351, 9, 25, 23, 0, 0, /
000039      DATA RHOS, /64, 64, /
000040      DATA RHOSB/3, 45, 6, 36, 9, 45, 23, 0, 0, /
000041      DATA SK/0, 0, 2, 0, 8, 5, 8, 5, 11, 6, 5, 8, 8, 0, 8, 23, 0, 0, /
000042      C COOLANT PROPERTIES
000043
000044      DATA AVC / 41, 100, /
000045      DATA CPC/41, 1, E20/
000046      DATA NOG / 1 /
000047      DATA T268 / 70, /
000048      DATA UC/41, 0, 0, /
000049      C HEAT TRANSFER COEFFICIENTS
000050
000051      DATA HSG / 41, 3, 0, /
000052      DATA HXC/13, 0, 2, 7, 3, 3, 3, 7, 23, 0, 0, /
000053      DATA HXG/18, 0, 0, 151, 23, 0, 0, /
000054      DATA HXS/3, 0, 55, 6, 79, 5, 9, 55, 23, 0, 0, /
000055      C MASS TRANSFER PROPERTIES
000056
000057      DATA DIF/41, 4, E-4/
000058      DATA GK/8, 5, E-4, 3, 0, 0, 0, 7, 1, E-3, 23, 0, 0, /

```



```

C PROCESS GAS STREAM PROPERTIES
C   DATA CPG / 41*0.23 /
   DATA DW / 11*400., 7*1400., 23*0.0 /
   DATA WM / 44.0, 18.0 /
C HX CORE 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

```

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ELT S9992,1.690501, 43774

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000001 FUNCTION PKEQ(ID,W,T)
000002 PKEQ=EQUILIBRIUM PRESSURE IN MM HG
000003 ID=2.420 ON 13X
000004 ID=1.002 ON MOLECULAR SIEVE 5A
000005 W=LOADING IN LB ADSORBATE PER LB ADSORBENT
000006 T=TEMP IN DEG F
000007 DATA 81/.0705230784 /
000008 DATA 82/.0422820123 /
000009 DATA 83/.0092705272 /
000010 DATA 84/.0001520143 /
000011 DATA 85/.0002765672 /
000012 DATA 86/.0000430638 /
000013 C
000014 IF (W .LE. 0.) W=1.E-5
000015 GO TO (41,51),ID
000016 41 CONTINUE
000017 Y=ALOG(W)
000018 YB1G=0.667*Y+2.22+0.0025*Y
000019 H=ABS(YB1G)
000020 IF (H .GE. 1.0) GO TO 231
000021 IF (H .LE. 0.984) GO TO 2
000022 IF (H .LE. 0.997) GO TO 5
000023 X0=2.2+200.*(H-0.998)
000024 GO TO 6
000025 16 CONTINUE
000026 IE(H .LE. 0.84) GO TO 1
000027 IF (H .LE. 0.88) GO TO 2
000028 IF (H .LE. 0.934) GO TO 3
000029 IF (H .LE. 0.984) GO TO 5
000030 IF (H .LE. 0.997) GO TO 5
000031 X0=2.2+200.*(H-0.998)
000032 GO TO 6
000033 231 H=1.0
000034 GO TO 17
000035 1 X0=H
000036 GO TO 6
000037 2 X0=1.0
000038 GO TO 6
000039 3 X0=1.2
000040 GO TO 6
000041 8 X0=1.3+8.*(H-.934)
000042 GO TO 6
000043 5 X0=1.7+30.*(H-.984)
000044 6 HPRXD=(2.7177245)*EXP(-1.*(X0)**2)
000045 C=-16.
000046 HNEW=1.+X0*(81+X0*(82+X0*(83+X0*(84+X0*(85+X0*(86))))))
000047 HNEW=1.-HNEW**C
000048 DELH=H-HNEW
000049 TERM=DELH/HPRXD
000050 XB1G=X0+TERM+X0*TERM**2*((4.+X0**2+1.)**TERM**3)/3.+(7.*X0**2.
000051 1*X0**3)**TERM**4/6.
000052 GO TO 18
000053 17 XB1G=4.0
000054 18 XB1G=SIGN(XB1G,YB1G)
000055 12 X=(XB1G-0.493+0.00953*T)/0.38
000056 PKEQ=EXP(X)
000057 RETURN
000058 51 CONTINUE
000059 PKEQ=EXP(47.2*W-1.31E4/(T+460.))+15.2)

```



322551

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	PR20, 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	76.0612
7	5.9285	.0266	76.1422	76.1446	69.9999	75.8128
8	6.5029	.0266	75.8939	75.8965	69.9999	75.4556
9	6.8842	.0266	75.6331	75.6358	69.9999	73.9867
10	6.8842	.0266	75.3529	75.3643	69.9999	73.0152
11	6.8842	.0266	73.7137	73.7079	69.9999	72.6148
12	6.8842	.0266	74.5609	74.5223	69.9999	72.8505
13	6.8842	.0758	80.1246	79.9936	69.9999	73.5828
14	6.8842	3.435	99.0533	98.8847	69.9999	73.3740
15	6.8842	2.2727	123.5286	123.5868	64.9999	73.2868
16	6.8842	5.7285	118.0636	118.1970	64.9999	72.5691
17	6.8842	7.5100	99.6914	99.8366	64.9999	72.6581
18	6.8842	8.8361	76.9300	79.1171	69.9999	

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB AXIAL NODE	1	2	3	4	5	6	7	8	9	10	11
1	.0356	.0357									
2	.0369	.0370									
3	.0385	.0386									
4	.0408	.0409									
5	.0433	.0434									
6	.0466	.0467									
7	.0506	.0507									
8	.0591	.0592									
9	.0010	.0010									
10	.0010	.0010									
11	.0010	.0010									
12	.1198	.1198									
13	.1364	.1365									
14	.1507	.1508									
15	.1708	.1710									
16	.1948	.1949									
17	.2162	.2163									
18	.2388	.2388									

AVG CO2 LOADING IN M.S. BED = .0426 LB/LB AVG H2O LOADING IN S.G. BED = .1753 LB/LB

TIME AVG CO2 ADSORP RATE = .2769 LB/HR TIME AVG H2O ADSORP RATE = .2482 LB/HR



TIME AVG EXIT PH2O = .0261 MS 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	64.8264	64.9259	69.9999	64.7709
4	1.7261	65.0595	65.0596	69.9999	65.2339
5	1.6884	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	65.6368
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	78.0094	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	15.6455	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	AVG	1	2	3	4	5	6	7	8	9	10	11
AXIAL NODE												
1	.0323	.0323	.0322									
2	.0327	.0328	.0326									
3	.0338	.0339	.0337									
4	.0355	.0354	.0352									
5	.0328	.0329	.0327									



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

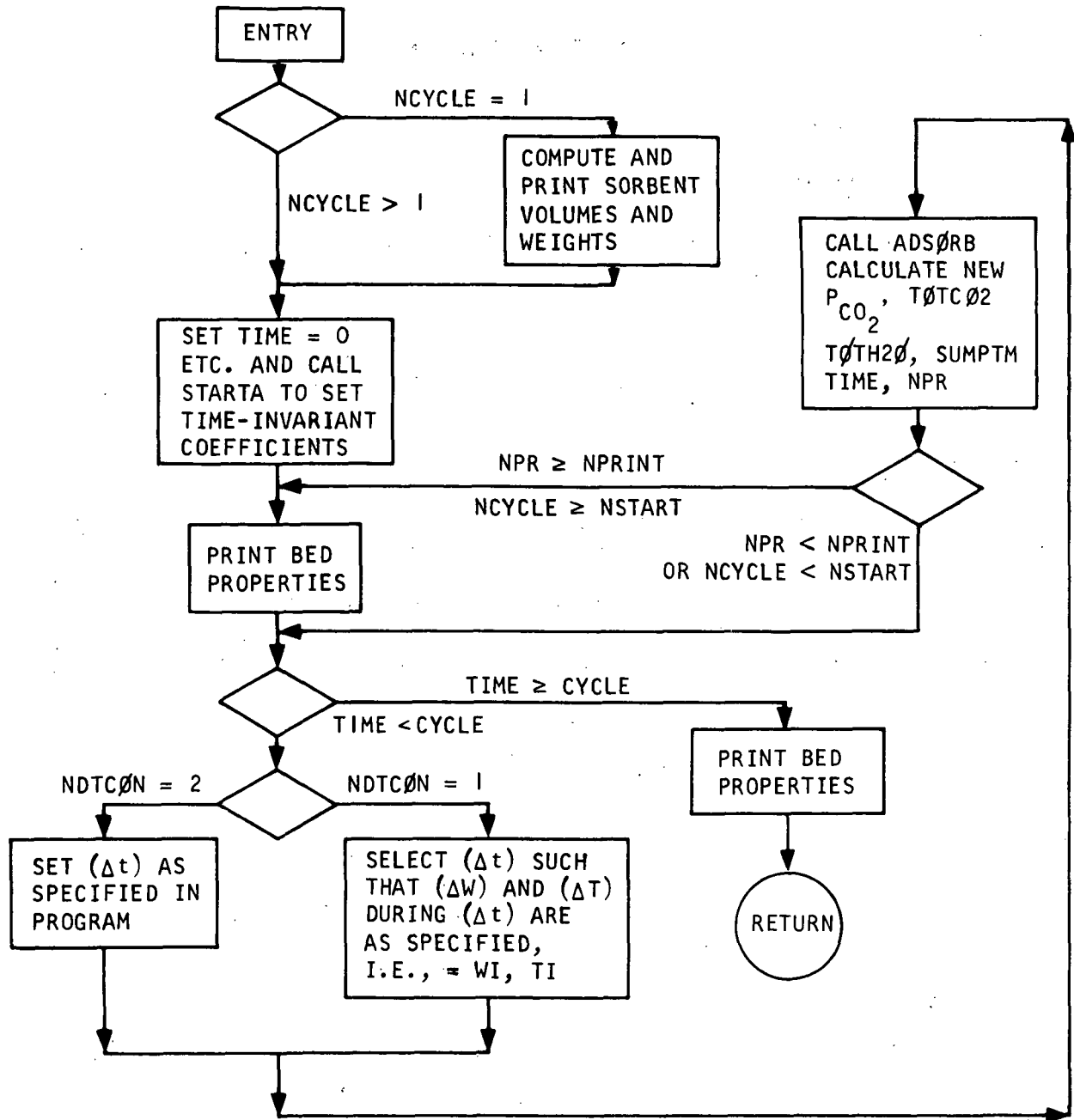
ADSORB (S9971)

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)

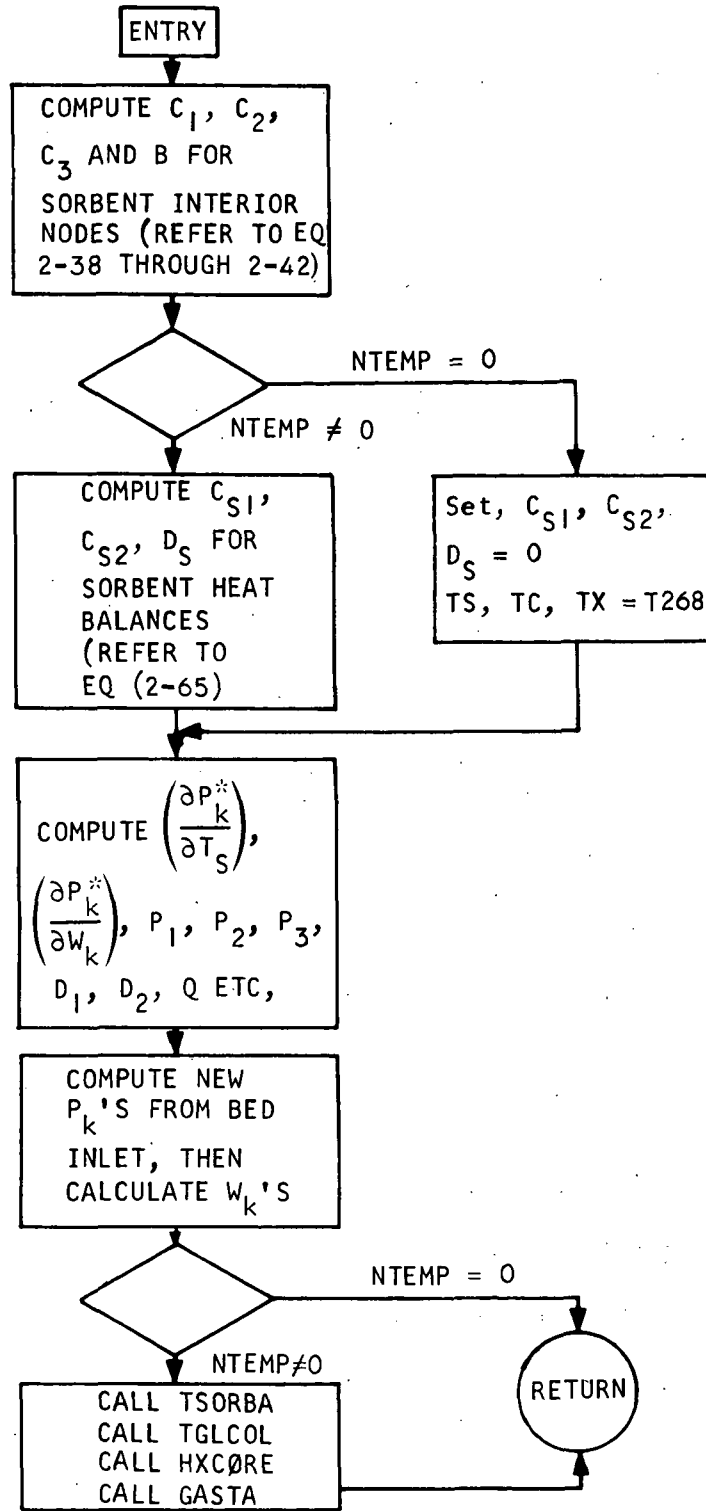
This routine solves Equation (2-32) for adsorption period sorbent temperatures, using the method shown in Equations (2-38) through (2-46).





S-50348

Figure 5-1. Logic Flow Chart for MADSOR



S-50349

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)(°F)

ABED = cross-sectional area, (sq ft)

NDXI = total number of axial nodes

TGI = process gas inlet temperature, °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) (°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) (°F)

DX = axial increment size, ft

TG = gas temperature, °F

TS = sorbent temperature, °F

TX = heat exchanger temperature, °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.

DESORB (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.

TSORB (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

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

CPG = specific heat of vapor mixture, Btu/(lb)(°F)

U = linear velocity of vapor mixture, ft/hr

TS = sorbent temperature, °F

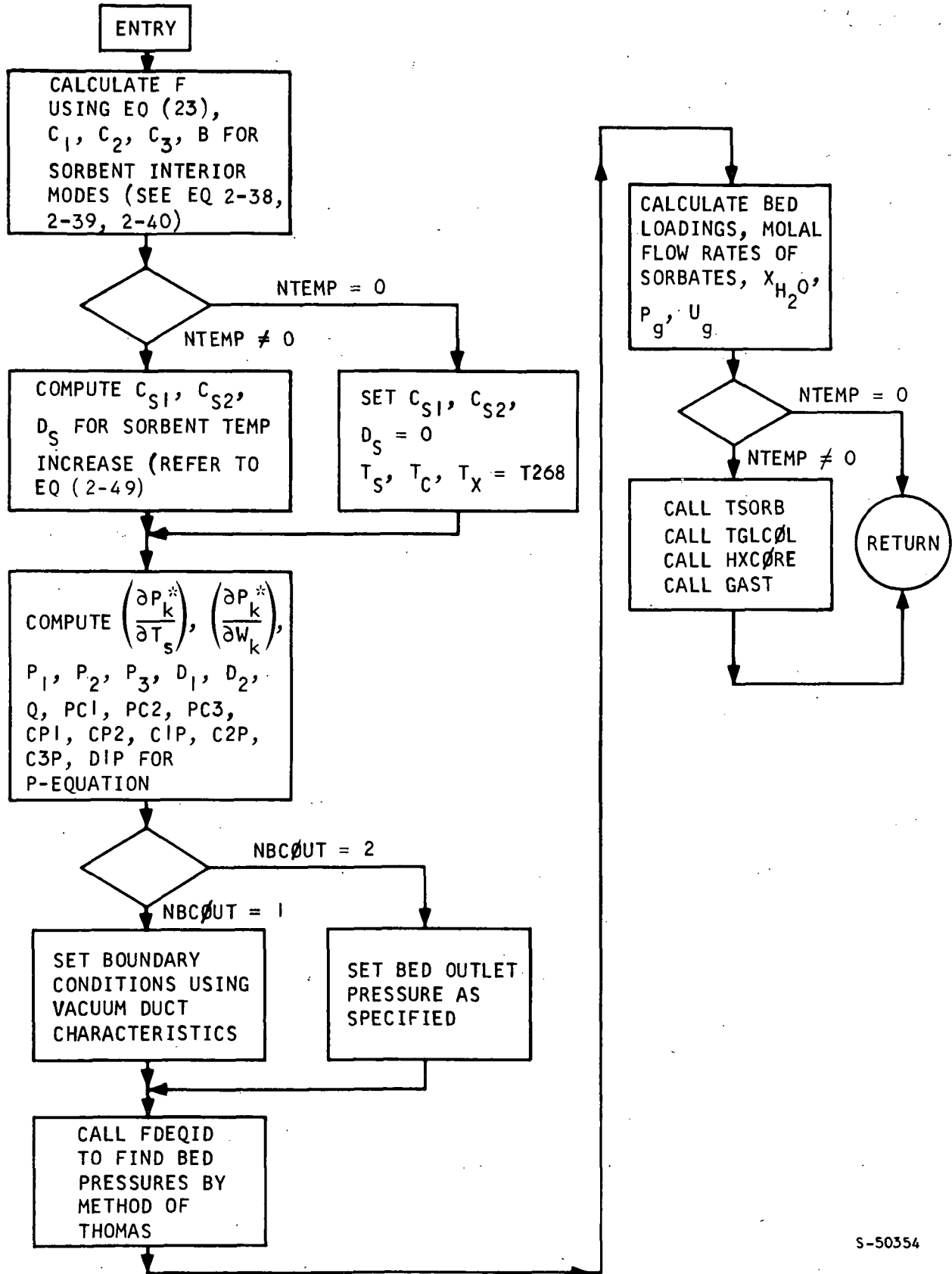
TX = heat exchanger temperature, °F

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)(°F)





S-50354

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)(°F)

TG = gas temperature, °F

$V\phi$ IDF = void fraction

PKEQ (S9992)

This function subprogram calculates the equilibrium CO₂ and H₂O vapor pressures over the molecular sieve and desiccant sorbents, respectively.

Arguments of the function are

ID = control index, ID = 1 indicates CO₂ over molecular sieve sorbent, ID = 2 indicates H₂O over desiccant sorbent.

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

T = sorbent temperature, °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



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

$X\phi$ = value of independent variable X

$Y\phi$ = value of dependent variable corresponding to $X\phi$ (this is the
answer obtained by LAGIN2)

Y = dependent variable



SOURCE PROGRAM LISTING



ELT S9960.1.690501, 43778

```

000001 C MAIN PROGRAM FOR COMBINED ADSORPTION/DESORPTION PROGRAM -- DEVELOPED
000002 C BY K C HWANG, AIRESEARCH , LOS ANGELES
000003 C
000004 COMMON /BLOK3/ W(21,41),TG(41),TS(41),TC(41),TX(41),CYCLE
000005 DOUBLE PRECISION W
000006 COMMON /BLOK6/ NCYCLT
000007 COMMON /BLOK14/ NCYCLE
000008 NCYCLE=1
000009 11 CONTINUE
000010 WRITE (6,300)
000011 CALL MADSOR
000012 WRITE (6,400)
000013 CALL MDESCR
000014 NCYCLE=NCYCLE+1
000015 IF(NCYCLE .LE. NCYCLT) GO TO 11
000016 CALL EXIT
000017 300 FORMAT(24H1 START ADSORPTION CYCLE.)
000018 400 FORMAT(24H1 START DESORPTION CYCLE.)
000019 .END

```



• ELT S9950.1.690501. 43776

CALL MADSOR
END

000001
000002



* ELT S9951.1.690501. 43777

CALL MDESOR
END

000001
000002



* ELT S9970.1.690501, 43780

```

000001 SUBROUTINE MADSOR
000002 C
000003 COMMON /BLOK2/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000004 1HXG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS(2), DVS1(2), R
000005 2S1(2,41), RHOS(2), AUG(41), WM(2), UC(41), NDM, PS(41), RHOSB(41), DS(41),
000006 3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000007 41), PC3(41), ASG(41), ASX(41), AGX(41), G1P(41), C2P(41), C3P(41), D1P(41)
000008 5, FR(2,41), RS(2), NDX1, NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
000009 6, P3(41), WS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000010 7(2,2,41), CP1(41), CP2(41), Y(41), VOIDF(41), TTIME
000011 8, AXG(41), RHOC(41), CPC(41), T268, AVX(41), TAX(41), CPX(41), RHOX(41),
000012 9, NOC, PK(2,41), PCO21, PH2O1, GMR, GMW, TGI, PA, PT(41), CPS(41), MSG(41)
000013 COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
000014 DOUBLE PRECISION W
000015 COMMON /BLOK8/ DTO, TS1(41), TS2(41), TX1(41), TX2(41), TC1(41), TC2(41)
000016 COMMON /BLOK10/ NPRINT, DTMAX, NDTCON
000017 COMMON /BLOK11/ TOTCO2, TOTR20, SUMPTM, WTACMS, WTSG
000018 COMMON /BLOK13/ W1, Y1
000019 COMMON /BLOK14/ NCYCLE
000020 COMMON /BLOK16/ NDXMAC, PCO2C, VOLCAB, RC02C
000021 COMMON /BLOK17/ NSTART
000022 C
000023 IF(NCYCLE .GT. 1) GO TO 1
000024 N1=NDXM+1
000025 VMS = 0.0
000026 VSG=0.0
000027 WTSG=0.0
000028 IF(NDXM .EQ. 0) GO TO 11
000029 DO 10 N= 1, NDXM
000030 VMS=VMS+DX*ABED(N)
000031 WTMS=WTMS+DX*ABED(N)*RHOSB(N)
000032
000033 10 CONTINUE
000034 11 IF((NDX1-NDXM).EQ. 0) GO TO 31
000035 DO 30 N= N1, NDX1
000036 VSG=VSG+DX*ABED(N)
000037 WTSG=WTSG+DX*ABED(N)*RHOSB(N)
000038
000039 30 CONTINUE
000040 31 CONTINUE
000041 WRITE(6,500) VMS, WTMS, VSG, WTSG
000042 500 FORMAT( 28H1TOTAL VOLUME OF M.S. BED = G10.4,2X,5HCU FT//
000043 123H TOTAL WT OF M.S. BED = G10.4,2X, 2HLB//
000044 228H TOTAL VOLUME OF S.G. BED = G10.4,2X,5HCU FT//
000045 323H TOTAL WT OF S.G. BED = G10.4, 2X,2HLB)
000046 WTACMS=0.0
000047 IF(NDXMAC .EQ. 0) GO TO 12
000048 DO 70 N= 1, NDXMAC
000049 70 WTACMS=WTACMS + DX*ABED(N)*RHOSB(N)
000050 12 CONTINUE
000051 WRITE(6,501) WTACMS
000052 501 FORMAT( / 30H TOTAL WT OF ACTIVE M.S. BED = , G10.4,3H LB )
000053 1 TIME = 0.0
000054 SUMPTM=0.
000055 DT = 1.E-5
000056 DTO = 0.0
000057 TOTCO2=0.0
000058 TOTR20=0.0

```





```

000059 DC 20 N=1,NDX1
000060 TS1(N)=TS(N)
000061 TS2(N)=TS(N)
000062 TX1(N)=TX(N)
000063 TX2(N)=TX(N)
000064 TC1(N)=TC(N)
000065 TC2(N)=TC(N)
000066
000067 20 CONTINUE
000068 CALL START
000069 NPR=NPRINT - 1
000070 GO TO 3
000071 2 CALL PRADSB
000072 NPR = 0
000073 4 CONTINUE
000074 IF( TIME .GE. CYCLE) CALL PRADSB
000075 IF( TIME .GE. CYCLE) GO TO 9999
000076 DT0=DT
000077 GO TO (41,42),NDTCN
000078 41 ADT=DTMAX
000079 DO 60 N=1,NDX1
000080 ADT2=1 / (ABS(W(NDR4,N))-WS(N))*1.E-9)*DT
000081 IF(ADT2.LT. ADT) ADT=ADT2
000082 ADT2=1 / (ABS(TS(N)-TS2(N))*1.E-9)*DT*2.0
000083 IF(ADT2.LT. ADT) ADT=ADT2
000084 ADT2=1 / (ABS(TX(N)-TX2(N))*1.E-9)*DT*2.0
000085 IF(ADT2.LT. ADT) ADT=ADT2
000086 ADT2=1 / (ABS(TC(N)-TC2(N))*1.E-9)*DT*2.0
000087 IF(ADT2.LT. ADT) ADT=ADT2
000088 60 CONTINUE
000089 DT=ADT
000090 GO TO 3
000091 42 DT=DTMAX/10.0
000092 IF( TIME .GT. 0.06) DT=DTMAX
000093 3 CONTINUE
000094 IF( TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
000095 DO 21 N=1,NDX1
000096 TS2(N)=TS1(N)
000097 TX2(N)=TX1(N)
000098 TX1(N)=TX(N)
000099 TC2(N)=TC1(N)
000100 TC1(N)=TC(N)
000101 21 CONTINUE
000102 PC021 = PC02C
000103 CALL ADSORB(DT)
000104 DPC02C = DT*(RC02C - GMR
000105 (PC021-PK(1,1))*44./((PA*GMW)*554.*530./((44.*
000106 2VOLCAB)
000107 PC02C=PC02C+DPC02C
000108 TOTC02=TOTC02+GMR*DT*(PC021-PK(1,1))*44./((PA*GMW)
000109 TOTX20=TOTX20+GMR*DT*(PH201-PK(2,1))*18./((PA*GMW)
000110 SUMPTIME=SUMPTM+PK(2,1)*DT
000111 TIME=TIME+DT
000112 NPR = NPR+1
000113 IF( (NPR.GE. NPRINT) .AND. (NCYCLE .GE. NSTART) ) GO TO 2
000114 GO TO 4
000115 9999 CONTINUE
000116 RETURN
000117 END

```

ELT S9971,1.690617, 53904 .1

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000001 SUBROUTINE ADSORB(DELT)
000002 COMMON /BLOK2/ ABED(41), A(41), AVC(41), CP6(41), RHOG(41),
000003 IHKG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS(2), DVS1(2), R
000004 251(2,41), RHOS(2), UG(41), WM(2), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000005 3G51(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000006 41), PC3(41), ASG(41), ASX(41), AGX(41), CIP(41), C2P(41), C3P(41), OIP(41)
000007 5, FR(2,41), RS(2), NDX1, NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
000008 6, P3(41), WS(41), CRI(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000009 7G(21,41), CPI(41), CP2(41), X(41), VOIDF(41), TIME
000010 8, AX(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41)
000011 9, NOG, PK(2,41), PCO21, PH2O1, GMR, CMW, TGI, PA, PT(41), CPS(41), HSG(41)
000012 COMMON /BLOK3/ W(21,41), TG(*1), TS(41), TC(41), TX(41), TX1(41), TC1(41), TC2(41)
000013 DOUBLE PRECISION W
000014 COMMON /BLOK8/ DTD, TS1(41), TS2(41), TX1(41), TX2(41), TX3(41), TC1(41), TC2(41)
000015 COMMON /BLOK12/ NTEMP
000016 DIMENSION AS(2)
000017 EQUIVALENCE (ASX,AS), (AGX,AXG), (ASG,AGS), (HXS,HSX), (HXG,HGX), (HSG
000018 1,HGS)
000019 DT = DELT
000020 AS(1)=4.*3.1416*RS(1)**2
000021 AS(2)=4.*3.1416*RS(2)**2
000022
000023
000024
000025 DATA RGAS/554./
000026
000027 NDR=NDR4-1
000028 DO 21 N=1,NDX1
000029 I=IFN(N,NDXM)
000030 DO 20 NR=1,NDR4
000031 C1(NR,N)=CR1(I,NR)/DT*CR2(I,NR)*CR3(I,NR)
000032 C2(NR,N)=CR1(I,NR)/DT*CR2(I,NR)*CR3(I,NR)
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* ELT S9970,1,690501, 43783

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000001 SUBROUTINE GASTA(CMR,CPG,ABED,NDX1,TGI,ASC,HSG,AXG,HXC,DX,TG,TS,TX
000002 1)
000003 C G4S TEMPERATURE CALCULATIONS FOR ADSORPTION
000004 C DIMENSION CPG(1),ASG(1),HSG(1),HXC(1),TG(1),TS(1),TX(1),ABED(1),
000005 1,AXG(1)
000006 C
000007 TG(NDX1+1) = TGI
000008 DO 10 N=1,NDX1
000009 N1=NDX1+1-N
00010 C=CMR*CPG(N1)/ABED(N1)
00011 C1=ASC(N1)*HSG(N1)*AXG(N1)+HXC(N1)
00012 10 TG(N1) = (TG(N1+1)/DX*(ASC(N1)*HSG(N1)+TS(N1)+AXG(N1)
00013 +HXC(N1)*TX(N1)) /
00014 1C)/(1./DX+C1/C)
00015 RETURN
00016 END
00017
00018

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e-ELT-99977,1,690501, 43786

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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
2SI(2,41), RHOS(2), UG(41), WML(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), CJP(41), C2P(41), CJP(41), D1P(41)
5, FR1(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), C1(41), CP2(41), X(41), VO1DF(41), TIME
8, AXEL(41), BMDL(41), CPC(41), Z268, AVX(41), JAX(41), CBX(41), RMOX(41)
9, N06, PK(2,41), PC021, PH201, GMR, GMW, TGI, PA, PT(41), CPS(41), HSG(41)
COMMON /BLOK3/ W(21,41), TG(41), TS(41), TC(41), TX(41), YX(41), CYCLE
DOUBLE PRECISION W
COMMON /BLOK4/ DT0, IS1(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+DT0)/CPS(N)/RHOSB(N)
11B1,S1,T*(ASG(N)+HSG(N)+ASX(N)+HXS(N))
CS1(N)=CS1(N)*(1.0+T)
CS2(N)=CS2(N)*(1.0+T)
1=1FN(N, NDXM)
TGAVG1=IG(N)
B1(N)=TS2(N)+CS1(N)*
1PK(1,N)
2
3PK(1,N)*
-CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)+WS(N))*
)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)=S1(N)-S3(N)+T1
10 CONTINUE
CALL EDEQIM(S1,S2,S3,B1,TS,NDX1)
RETURN
END

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ELT S9978,1.690501, 4378c

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000001 SUBROUTINE STARTA
000002 C
000003 COMMON /BLOK2/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000004 1HXC(41), HXS(41), HXC(41), DJF(41), F(41), C(41), VS(2), DVS(2), DVS1(2), R
000005 2S1(2,41), RHOS(2), UG(41), WM(2), UC(41), NDXM, BS(41), RHOSB(41), DS(41),
000006 3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000007 41), PC3(41), ASE(41), ASX(41), AGX(41), C1R(41), C2P(41), C3P(41), D1R(41)
000008 5, FR(2,41), RS(2), NDX1, NDR, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
000009 6, P3(41), WS(41), CRI(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000010 7Q(21,41), CP1(41), CP2(41), X(41), VOIDF(41), TIME
000011 8, AXG(41), RHOC(41), CFC(41), T288, AVX(41), TX(41), CPX(41), RHGX(41),
000012 9, NQG, PK(2,41), PCO21, PH201, GMR, GMW, TGI, PA, PT(41), CPS(41), HSG(41)
000013 COMMON /BLOK3/ W(21,41), TC(41), TS(41), TC(41), TX(41), CYCLE
000014 DOUBLE PRECISION W
000015 DO 115 N=1, NDX1
000016 115 A(N)= GMR/ABED(N)/PA/GMW
000017 C
000018 C
000019 RS(1)=RHOS(1)*3./RHOS(1)/ASC(1)
000020 RS(2)=RHOSB(NDX1)
000021 1 NDR=NDR4-1
000022 NDR2=2.*NDR
000023 NDR3=NDR2+1
000024 DO 10 I=1,2
000025 VS(I)=4./3.*3.1416*RS(I)**3
000026 DVS(I)=VS(I)/NDR
000027 DVS1(I)=DVS(I)/2
000028 RS1(I)=0.
000029 DO 10 K=2, NDR3
000030 10 RS1(I,K)=CBRT(3./4.*3.1416*(4./3.*3.1416*RS1(I,K-1)+DVS1(I)))
000031 DO 11 I=1,2
000032 IF(I.EQ.1) DJF=DJF(1)
000033 IF(I.EQ.2) DJF=DJF(NDX1)
000034 CRI(1,1)=DVS1(1)/RHOS(1)
000035 CRI(1,1)=0.
000036 CRI(1,1)=4.*3.1416*RS1(1,2)*2*DJF1 /RS1(1,1)+RHOS(1)
000037 DO 11 K=2, NDR4
000038 CRI(1,K)=DVS(1)/RHOS(1)
000039 CRI(1,K)=4.*3.1416*RS1(1,2)*K-2)*2*DJF1 /RS1(1,2)*K-1)-RS1(1,2)*K-1)
000040 13) *RHOS(1)
000041 11 CRI(1,K)=4.*3.1416*RS1(1,2)*K)*2*DJF1 /RS1(1,2)*K-1)-RS1(1,2)*K-1)
000042 1) *RHOS(1)
000043 CRI(1,NDR4)=CRI(1,1)
000044 CRI(2,NDR4)=CRI(2,1)
000045 RETURN
000046 END

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e-ELI-59979.1.690501.43767

SUBROUTINE PRADSB

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C
C
DIMENSION AVLD(41)
COMMON /BLOK2/ ABED(41), A(41), AVC(41), CPG(41), RH05(41),
1HXG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS(2), R
2S1(2,41), RHOS1(2), UC(41), WM(2), UC(41), ANDXM, PS(41), RHOSB(41), DS1(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), CLP(41), C2P(41), C3P(41), DJP(41)
5, FR(2,41), RS(2), NDX1, NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
6, P3(41), MS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
70(21,41), CPI(41), X(41), X(41), VOIDF(41), TIME
8, AX(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41)
9, NOG, PK(2,41), PC021, PM201, GMR, CMW, TG, 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), TIME1(10), NBCOUT, NPSET(3)
COMMON /BLOK5/ D10, IS1(41), TS2(41), TX1(41), TX2(41), TC1(41), TC2(41)
COMMON /BLOK6/ NCVCLY
COMMON /BLOK8/ D10, IS1(41), TS2(41), TX1(41), TX2(41), TC1(41), TC2(41)
COMMON /BLOK10/ NPRINT, DTMX, NDTCON
COMMON /BLOK11/ TOTCO2, TOTM20, SUMPTM, WTACHS, WTSG
COMMON /BLOK12/ NTEMP
COMMON /BLOK13/ M1, I1
COMMON /BLOK14/ NVCYCLE
COMMON /BLOK16/ NDXMAC, PC02C, VOLCAB, RC02C
COMMON /BLOK17/ NSTART
DIMENSION AXS1(41), AXG(41), AGS(41), HSX(41), HGX(41), HGS(41), ACX(41),
1HX(41)
EQUIVALENCE (ASX,AXS), (AGX,AXG), (ASG,AGS), (HSX,HSX), (HGX,HGX), (HSG
1,HGS), (AXC,ACX), (HXC,HXC)
EQUIVALENCE (NDX,NDX1)
AVPZ0 = SUMPTM/TIME
AVHZOP = GMR*AVPHZ0*18./(PA*CMW)

C
TIME=0., TIME
WRITE (6,100) NVCYCLE, TIME, TIMEH, DT
WRITE (6,101)
WRITE (6,102) (N,PK1,N),PK(2,N),
1 TG(N),T8(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=1, 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, NDR2
33 SUMMS=SUMMS+W(NR,N)

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000059 AVLD(N)=SUMMS/NDR3
000060 30 CONTINUE
000061 SUM#0.
000062 IF(NDXMAC.EQ.0) GO TO 35
000063 DO 31 NR 1, NDXMAC
000064 31 SUM# SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000065 AVMSLD # SUM/WTACMS
000066 SUM#0.
000067 35 CONTINUE
000068 IF((NDX1-NDXM).EQ.0) GO TO 40
000069 DO 32 NR N1,NDX1
000070 32 SUM # SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000071 AVMSLD=SUM/WTSC
000072 40 CONTINUE
000073 DO 30 NR 1,NDX
000074 30 WRITE (6,203)N, AVLD(N)
000075 ,LW(NR,N),NR#1,NDR4)
000076 WRITE (6,205) AVMSLD, AVMSLD
000077 AVRCO2=TOTCO2/TIME
000078 AVRH2O=TOTH2O/TIME
000079 WRITE(6,204) AVRCO2,AVRH2O.
000080 RETURN
000081 100 FORMAT (1M1.16H4DSORPTION CYCLE 13/
000082 3X.5HTIME#F9.5,3X2HHR,F12.3,1X,3MMIN,
000083 5X.15HTIME INCREMENT#F7.5,3X2HHR)
000084 101 FORMAT (//2X,10MAXIAL NODE#3X,3MRCO2,MM,5X,7M20,MM,4X,
000085 1X,GAS TEMP, F
000086 1X,15MSORBENT TEMP, F
000087 1X,15MCOOLANT TEMP, F
000088 2RE TEMP, F )
000089 102 FORMAT (//19.2F12.4,5X,4(F(4.4,4X)))
000090 202 FORMAT (// 36HOLADING AT INTERIOR OF SORBENT, LB/LB
000091 //4X,4HSORB/4X,4HNOO
000092 1E.3X, 3HAVG, 9X,
000093 1 1H1.9X,1M2.9X,1M3.9X,1M4.9X,1M5.9X,1M6.9X,1M7.9X,
000094 21H6.9X,1H9.9X,2H10,
000095 28X,2H11/6H AXIAL/5H NODE)
000096 203 FORMAT ( 15.4X,12(F6.4,4X))
000097 204 FORMAT (//27H0TIME AVG CO2 ADSORP RATE #
000098 1 F6.4, 6H LB/HR ,10X,
000099 3 F6.4, 7H LB/HR
000100 205 FORMAT (// 30H AVG CO2 LOADING IN M.S. BED # F8.4,1X,5HLB/LB,7X,
000101 130H AVG H2O LOADING IN S.G. BED # F8.4, 6H LB/LB)
000102 206 FORMAT (//21H TIME AVG EXIT RH2O # F10.4, 1X,MM ,18X,
000103 140H TIME AVG RATE OF M.S. POISONING BY H2O # G12.4,10H LB H2O/HR)
000104 END
000105

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@ ELT S9980.1.690501. 43789

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000001 SUBROUTINE MDESOR
000002 MAIN PROGRAM FOR TRANSIENT DESORPTION BED CALCULATIONS
000003 C
000004 C
000005 COMMON /BLOK1/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000006 1HXG(41),HXG(41),MXC(41),DIF(41),E(41),C(41),VS(2),DVS(2),DVS1(2),R
000007 2S1(2,41),RHOS(2),UG(41),VM(2),UG(41),NDXM,PS(41),RHOSB(41),DS(41),
000008 3CS1(41),CS2(41),C1(21,41),C2(21,41),D1(21,41),D2(41),PC1(41),PC2(4
000009 41),PC3(41),ASG(41),ASX(41),AGX(41),C1P(41),C2P(41),C3P(41),D1P(41)
000010 5,FR(2,41),RS(2),NDX1,NDR4,DX,DT,CK(41),DH(41),SK(41),P1(41),P2(41),
000011 6,P3(41),WS(41),CRI(2,21),CR2(2,21),CR3(2,21),C3(21,41),B(21,41),
000012 7G(21,41),CPI(41),CPE(41),X(41),AVOIDE(41),TIME
000013 8,AXC(41),RHOC(41),CPCI(41),T268,AVX(41),TKX(41),CPX(41),RHOX(41)
000014 9,NOC,PK(2,41),PCO21,PU201, GMR,GMW,TGL,PA,PT(41),CPS(41),MSG(41)
000015 DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,G7B,
000016 1 C1,CP2,X,DT
000017 DOUBLE PRECISION C1P,C2P,C3P,D1P
000018 COMMON /BLOK3/ W1,21,41,TG(41),TS(41),TC(41),TX(41),CYCLE
000019 DOUBLE PRECISION W
000020 COMMON /BLOK6/ DIQ,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
000021 COMMON /BLOK10/ NPRINT,DTMAX,NDTCON
000022 COMMON /BLOK11/ TOTCO2,TOTHZO
000023 COMMON /BLOK13/ W1, T1
000024 COMMON /BLOK14/ NCYCLE
000025 COMMON /BLOK17/ NSTART
000026 TIME = 0.0
000027 DIQ = 0.0
000028 DT = 1.E-5
000029 TOTCO2 = 0.0
000030 TOTHZO = 0.0
000031 DO 20 N=1,NDX1
000032 TS1(N) = TS(N)
000033 TS2(N) = TS(N)
000034 TX2(N) = TX(N)
000035 TX1(N) = TX(N)
000036 TC1(N) = TC(N)
000037 TC2(N) = TC(N)
000038 20 CONTINUE
000039 CALL START
000040 CALL PROESB
000041 NPR = 0
000042 GO TO 3
000043 2 CALL PROESB
000044 IF( TIME .GE. CYCLE) GO TO 9999
000045 NPR = 0
000046 4 CONTINUE
000047 DT = DT
000048 GO TO (41,42),NDTCON
000049 41 ADI = DTMAX
000050 DO 60 N=1,NDX1
000051 ADT2 = 1 / (ABS(W(NDR4,N)) + WS(N)) + 1.E-9 * DT
000052 IF (ADT2.LT. ADT) ADT = ADT2
000053 ADT2 = 1 / (ABS( TS(N) - TS2(N)) + 1.E-9) * DT * 2.0
000054 IF (ADT2.LT. ADT) ADT = ADT2
000055 ADT2 = 1 / (ABS( IX(N) - IX2(N)) + 1.E-9) * DT * 2.0
000056 IF (ADT2.LT. ADT) ADT = ADT2
000057 ADT2 = 1 / (ABS( TC(N) - TC2(N)) + 1.E-9) * DT * 2.0
000058 IF (ADT2.LT. ADT) ADT = ADT2

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000059 60 CONTINUE
000060 DT=ADT
000061 GO TO 3
000062 42 DT=DTMAX/10.0
000063 IF(TIME .LT. 1.5E-4) DT=DTMAX/1000.0
000064 IF(TIME .GT. 0.06) DT=DTMAX
000065 3 CONTINUE
000066 IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
000067 DO 21 N=1,NDX1
000068 TS2(N)=TS1(N)
000069 IS1(N)=IS(N)
000070 TX2(N)=TX1(N)
000071 TX1(N)=TX(N)
000072 TC2(N)=TC1(N)
000073 TC1(N)=TC(N)
000074 21 CONTINUE
000075 D9=DI
000076 CALL DESORB(D9)
000077 TOTCO2=TOTCO2+DT*ER(1,NDX1)*MM(1)
000078 TOTH2O=TOTH2O+DT*FR(2,NDX1)*MM(2)
000079 TIME=TIME+DT
000080 NPR=NPR+1
000081 IF (NPR.GE. NPBINTL .AND. (NCYCLE..GE. NSYAFI)) GO TO 2
000082 IF(TIME .GE. CYCLE) GO TO 2
000083 GO TO 4
000084 9999 CONTINUE
000085 RETURN
000086 END

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@ ELT S9981.1.690501, 43789

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



ELT 59983,1,691016, 39084 , 1

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C
SUBROUTINE DESORB(DELTA)
COMMON /BLOK1/ ABED(41), A(41), AVC(41), CPCG(41), RHOG(41),
1HXG(41),HXG(41),HXG(41),DIF(41),F(41),C(41),VS(2),DVS(2),DVS1(2),R
2S1(2,41),RHOS(2),UG(41),WY(2),UC(41),NDXM,PS(41),RHOSR(41),DS(41),
3CSI(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),CIP(41),C2P(41),C3P(41),DIP(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),CRI(2,21),CR2(2,21),CR3(2,21),C3(21,41),R(21,41),
7G(21,41),CPI(41),CP2(41),X(41),VOIDF(41),TIME
8,AX(41),RHOC(41),CPC(41),T26R,AVX(41),TKX(41),CPX(41),RHGX(41)
9,NOG,PK(2,41),PCO2I,P420I, GMR,GMW,TG,PA,PT(41),CPS(41),HSG(41)
COMMON /BLOK8/ DTD,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,DPKDT5,
1DPKDK,CP1,CR2,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),P3(41)
DIMENSION P4(41),VIST(2)
DOUBLE PRECISION PD
DOUBLE PRECISION C1P,C2P,C3P,DIP
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
DATA RGAS/554./
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)
C3(NR,N)=-CR3(I,NR)
20
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
TO CALCULATE CS1,CS2,JS FOR SORBENT HEAT BALANCE EQUATION
IF(NTMP.EQ.0) GO TO 111
C

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000119 DO 25 N=2,NDX
000120 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1)
000121 1)/F(N+1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(2.*DX)
000122 N=1
000123 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1)
000124 1)/F(N+1) - VOIDF(N )*C(N )*ABED(N )/F(N ))/(1.*DX)
000125 N= NDX1
000126 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N )*C(N )*ABED(N
000127 1)/F(N ) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(1.*DX)
000128 DO 26 N=1,NDX1
000129 PC1(N)=PT(N)/F(N)
000130 PC3(N)=PT(N)/C(N)/VOIDF(N)*ASG(N)*GK(N)
000131 C
000132 DO 27 N=1,NDX1
000133 CP1(N)=PC3(N)*(PI(N)+2(N)*(Q(NDR4,N)-W(NDR4,N)))
000134 CP2(N)=PC3(N)*(P2(N)+2(N)*P3(N) -X(N))
000135 CIP(N)=-PC1(N)/DX+PC2(N)/2./DX
000136 C2P(N)=1./DT+2.*PC1(N)/DX+DX-C2(N)
000137 C3P(N)=-PC1(N)/DX+DX-C2(N)/2./DX
000138 DIP(N)=PT(N)/DT+CP1(N)
000139 C
000140 BOUNDARY CONDITION FOR P-EQUATION
000141 C
000142 C2P(1)=C2P(1)*CIP(1)
000143 CIP(1)=0.
000144 GO TO (55,56), NRCOUT
000145 55 CONTINUE
000146 PTNDX1=PT(NDX1)/D.888
000147 CEXIT=(ALOG(PTNDX1)+1.76)/(1.96*PT(NDX1))/(VOIDF(NDX1)*RHOG(NDX1)
000148 1 *ABED(NDX1))
000149 C2P(NDX1) = C2P(NDX1)+C3P(NDX1)*(1.-DX)*F(NDX1)*CEXIT)
000150 C3P(NDX1)=0.0
000151 GO TO 57
000152 56 CONTINUE
000153 C PRESSURES ARE SET
000154 C
000155 DO 561 K= 1, 3
000156 IF(NPSET(K) .EQ. 0) GO TO 561
000157 NP=NPSET(K)
000158 CIP(NP)=0.0
000159 C2P(NP)=1.0
000160 C3P(NP)=0.0
000161 CALL LAGIN2(10,TIMET,10,2,TIME,D1PNP ,POUT)
000162 DIP(NP)=D1PNP
000163 561 CONTINUE
000164 57 CONTINUE
000165 CALL F0EGID(C1P,C2P,C3P,D1P,PD,NDX1)
000166 DO 34 N=1,NDX1
000167 IF(PD(N) .LE. 0.) PD(N) = 1.E-3
000168 34 PT(N)=PD(N)
000169 C
000170 TO CALCULATE SORBENT LOADING
000171 C
000172 DO 30 N=1,NDX1
000173 W(NDR4,N)=Q(NDR4,N)+D2(N)*PT(N)
000174 DO 30 J=2,NUR4
000175 L=NDR4+1-J
000176 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
000177 30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
000178 C
000179 TO CALCULATE STREAM COMPOSITION
000180 C

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FR(1,1) = 0.0
FR(2,1) = 0.
FR2 = 0.0
DO 31 N=1,NDX1
I = IFN(N,NDX1)
TEMP = C(N)*VOIDF(N)
1/PA(N)*ABED(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(1,1) = TEMP
202 X(N) = 1.0
GO TO 31
201 CONTINUE
CT = ABED(N)*DX*ASC(N)*CK(N)
FRT = FR(1,N)+FR(2,N)+1.E-10
PSURF = P1(N)+P2(N)*4*(NDR4,N)-WS(N))*P3(N)*PT(N)
X(N) = ((FR(2,N-1)+CT*PSURF
1 (1+CT*PT(N)/FRT)
)/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,N)*WM(1)+FR(2,N)*WM(2))/RHOG(N)/ABED(N)/VOIDF(N)
33 CONTINUE
IF(NTEMP.EQ.0) RETURN
C TO CALCULATE SORBENT TEMPERATURES
CALL TSCRB
C
D9=DT
CALL TGLCOL(TG,NDX1,UC,RHOG,CPG,CX,AXG,HXG,T268,TX,DX,D9,AVC,MOG)
CALL HXCORE(TX,TC,TS,TG,HXC,HXS,HXG,RHOX,CPX,TKX,DX,D9,NDX1,AVX,
1NDXM)
CALL GAST(DX,RHOG,CPG,UC,TS,TX,NDX1,ASC,HSG,AXG,HXG,TC,VOIDF)
100 FORMAT(8G12.3)
RETURN
END
    
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C

C

C

100



ELT 5984.1.690501. 43794

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000001 SUBROUTINE FDEG(H(C1,C2+C3+O,VAR,NN)
000002 DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),O(41)
000003 NN1=NN-1
000004 B(1)=C3(1)/C2(1)
000005 DO 41 J=2,NN1
000006 41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000007 O(1)=D(1)/C2(1)
000008 DO 42 J=2,NN
000009 42 O(J)=(D(J)-C1(J)*O(J-1))/(C2(J)-C1(J)*B(J-1))
000010 VAR(NN)=O(NN)
000011 DO 43 J=2,NN
000012 L=NN+1-J
000013 43 VAR(L)=O(L)-B(L)*VAR(L+1)
000014 RETURN
000015 END

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• ELT S9285.1.690581, 43795

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000001 SUBROUTINE FDEQID(C1,C2,C3,D,VAR,NN)
000002 DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),O(41)
000003 DOUBLE PRECISION C1,C2,C3,D,VAR,B,O
000004 NN1=NN-1
000005      8(1)=C1(1)/C2(1)
000006 DO 41 J=2,NN1
000007     41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000008     8(1)=D(1)/C2(1)
000009     DO 42 J=2,NN
000010     42 O(J)=(O(J)-C1(J)*O(J-1))/(C2(J)-C1(J)*B(J-1))
000011     VAR(NN)=B(NN)
000012     DO 43 J=2,NN
000013     L=NN+1-J
000014     43 VAR(L)=O(L)-B(L)*VAR(L+1)
000015 RETURN
000016 END
    
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• ELI 59986.1.690501. 43796

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000001 .SUBROUTINE GAST (DX,RHOG,CPO,U,TS,TX,NDX1,ASG,HSC,AXG,HXG,TG,VOIDF
1)
000002 DIMENSION RHOG(1),CPO(1),U(1),TS(1),TX(1),TG(1),ASG(1),HSC(1),HXG(
000003 1),VOIDF(1),AXG(1)
000004 W=1.0
000005 N2= NDX1-1
000006 IZ(1)=IS(1)
000007 DO 10 N= 1, N2
000008 E= 0.5*(VOIDF(N)+ VOIDF(N+1))
000009 AS1=ASC(N+1)
000010 H81=HSC(N+1)
000011 AX1=AXG(N+1)
000012 HX1=HXG(N+1)
000013 CPl=CPC(N)
000014 RO= 0.5*(RHOG(N)+RHOG(N+1))
000015 U1= 0.5*( U(N)+U(N+1))
000016 TS1=TS(N+1)
000017 TX1=TX(N+1)
000018 C1=1./(F+RO*CPI*U1)
000019 D=C1*(AS1*H81*TS1+AX1*HX1*TX1)
000020 AS1(AS1*H81*AX1*HX1)*C1
10 TG(N+1)=((1./DX)*A*(1.-W))+TG(N)+D/(1./DX+A*W)
000021
000022
000023
000024 END

```



* ELI 59887,1,090501,43797

```

000001 SUBROUTINE TGLCOL(TC,NDXMAX,UC,RHOC,CPC,CX,AXC,MXC,T268,TX,DX,DT,
000002 1AVC, NOGLIN)
000003 DIMENSION C1(41),C2(41),C3(41),D(41),D(41),TC(1),TX(1),HXC(1),AVC(1),B(4
000004 11),Q(41)
000005 DIMENSION UC(1),RHOC(1),CPC(1),AXC(1)
000006 COMMON /BLOK6/ DTD,TS1(4),TS2(4),TX1(4),TX2(4),TC1(4),TC2(4)
000007 DMSDI=DTD
000008 DO 10 N= NOGLIN,NDXMAX
000009 C11=-UC(N)
000010 CC2=HXC(N)/(CPC(N)*RHOC(N))*AVC(N)*0.5
000011 IF( UC(N) .GT. 0.1 GO TO 5
000012 C3(N)=CC1/DX
000013 C2(N)=1./DN+CC2-C3(N)
000014 C1(N)=0.0
000015 GO TO 10
000016 5 C1(N) = CC1/DX
000017 C2(N) = 1./DN + CC2 - C1(N)
000018 C3(N) = 0.0
000019 10 Q(N)=C2(N)/DN+CC2+X1(N)*2. - CC2+TC2(N)
000020 C1(NOGLIN) = 0.
000021 C1(NOGLIN) = 0.
000022 D(NOGLIN)=D(NOGLIN) +ABS(UC(NOGLIN))/DX*T268
000023 NOG2=NOGLIN-1
000024 DO 51 N= 1, NOG2
000025 51 TC(N)=D.DD
000026 NN=NDXMAX
000027 NN1=NN-1
000028 N1=NOGLIN
000029 N2=N1+1
000030 B(N1)*C3(N1)/C2(N1)
000031 DO 41 J=N2,NN1
000032 41 B(J)=C3(J)/C2(J)+C1(J)*B(J-1)
000033 B(N1)=B(N1)/C2(N1)
000034 DO 42 J=N2,NDXMAX
000035 42 B(J)=D(J)+C1(J)*B(J-1)/C2(J)+C1(J)*B(J)
000036 TC(NN)=Q(NN)
000037 DO 43 J=N2,NN
000038 L=NN*N1-J
000039 43 TC(L)=Q(L)-B(L)*TC(L+1)
000040 RETURN
000041 END

```



ELT 5998A-1-490617, 53903

SUBROUTINE START

```

000001 COMMON /BLOK1/ ABED(41), A(41), AVC(41), CP6(41), RMO6(41),
000002 1HXG(41), HXS(41), HVC(41), DIF(41), F(41), C(41), VS(2), DVS(2), DVS1(2), R
000003 2SIF(2,41), RHOS(2), UC(41), WHI(2), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000004 3CS1(41), CS2(41), C1(21,41), C8(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000005 41), PC3(41), ASG(41), ASX(41), AGX(41), CSP(41), C2P(41), C3P(41), D1P(41)
000006 5, FR1(2,41), RS(2), NDX1, NDR4, DX, DT, GK(41), DM(41), SK(41), PI(41), P2(41)
000007 6, P1(41), H5(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000008 7(21,41), CP1(41), CP2(41), X(41), VOIDF(41), TIME
000009 8, AX(41), RHOC(41), CPC(41), T268, AVX(41), TKX(41), CPX(41), RHOX(41)
000010 9, NOG, PK(2,41), PCO21, PM201, GMR, GMW, TGI, PA, PT(41), CPS(41), HSG(41)
000011 DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, P1, P2, P3, Q, B,
000012 1 CPI, CP2, X, DT
000013 DOUBLE PRECISION C1P, C2P, C3P, D1P
000014 COMMON /BLOK3/ V(21,41), TG(41), TS(41), TC(41), TX(41), CYCLE
000015 DOUBLE PRECISION H
000016
000017 C
000018 1ST NDX1=NDXM
000019 DMF=0.8/1ST
000020 RS(1)=RHOSB(1)/ABG(1)
000021 RS(2)=RHOSB(NDX1)
000022 1 23./RHOS(2)/ABG(NDX1)
000023 DO 30 N=1, NDX1
000024 RMOS(N)=0.0001
000025 X(N)=1.0
000026 IDEFN(N, NDXM)
000027 IS=N-NDXM
000028 IF(10.EQ.2) X(N)=IS*DMF
000029 C(N)=0.2E-3
000030 PT(N)=4.00
000031 1=IFN(N, NDXM)
000032 30 VOIDF(N)=1.-RHOS(N)/RHOS(1)
000033 X(NDXM+1)=0.01
000034 NDR=2, NDR
000035 NDR3=NDR2+1
000036 DO 10 I=1, 2
000037 VS(I)=4./3.*3.1416*RS(I)*e3
000038 DVS(I)=VS(I)/NDR
000039 DVS1(I)=DVS(I)/2
000040 RS1(I)=0.
000041 DO 10 K=2, NDR3
000042 10 RS1(I,K)=CBRT(3./4./3.1416*(4./3.*3.1416*RS1(I,K-1)*e3+DVS1(I)))
000043 DO 11 I=1, 2
000044 IF(1.EQ.1) DIF1=DIF(1)
000045 IF(1.EQ.2) DIF1=DIF(NDX1)
000046 CR1(I,1)=DVS1(I)*RHOS(1)
000047 CR2(I,1)=0.
000048 CR3(I,1)=4.*3.1416*RS1(I,2)*e2*DIF1 / (RS1(I,3)*RS1(I,1))*RHOS(1)
000049 DO 11 K=2, NDR4
000050 CR1(I,K)=DVS(I)*RHOS(I)
000051 CR2(I,K)=4.*3.1416*RS1(I,2)*e2*DIF1 / (RS1(I,2)*K-1)*RS1(I,2)*K
000052 13)*RHOS(I)
000053 11 CR1(I,K)=4.*3.1416*RS1(I,2)*e2*DIF1 / (RS1(I,2)*K-1)*RS1(I,2)*K-1
000054 1)*RHOS(I)
000055 CR1(1, NDR4)=CR1(1,1)
000056 CR1(2, NDR4)=CR1(2,1)
000057
000058

```



RETURN
END

000059
000060



* ELI-59989.1.690503> 43800

```

000001 SUBROUTINE PROESB
000002 C
000003 C
000004 DIMENSION AVLD(41)
000005 COMMON /BLOK1/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000006 1HXG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS1(2), R
000007 2SI(2,41), RHDS(2), UG(41), WK(2), UC(41), NDR4, PS(41), RHOSB(41), OS(41),
000008 3CS(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000009 41), PC3(41), ASG(41), ASX(41), AGX(41), C1P(41), C2P(41), C3P(41), D1P(41)
000010 5, FR(2,41), RB(2), NDX1, NDR4, DX, DT, GK(41), DH(41), SK(41), P1(41), P2(41)
000011 6, P3(41), WS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000012 7G(21,41), CPI(41), CP2(41), X(41), VOIDF(41), TIME
000013 8, AX(41), RMGC(41), CPC(41), T268, AVX(41), YKX(41), CRX(41), RMGX(41)
000014 9, NDS, PK(2,41), PCO21, PH201, GMR, GHW, TGI, PA, PT(41), CPS(41), HSG(41)
000015 COMMON /BLOK3/ W(21,41), T8(41), TS(41), TC(41), TX(41), CYCLE
000016 DOUBLE PRECISION W
000017 COMMON /BLOK4/ POUT(10), TIMEF(10), NBCOUT, NPSET(3)
000018 COMMON /BLOK6/ NCYCLT
000019 COMMON /BLOK7/ D10, TS(41), PS(41), TX1(41), TX2(41), TC1(41), TC2(41)
000020 COMMON /BLOK10/ NPRINT, DTMX, NOTCON
000021 COMMON /BLOK11/ TOTCO2, TOTM20, SUMPIM, VTACHS, JTSC
000022 COMMON /BLOK12/ NTEMP
000023 COMMON /BLOK13/ W, T1
000024 COMMON /BLOK14/ NCYCLE
000025 COMMON /BLOK16/ NDMAC, PCOBC, VOLCAB, RCO2C
000026 COMMON /BLOK17/ NSTART
000027 DIMENSION AXS(41), AXG(41), AGS(41), HBS(41), HCS(41), HGS(41), ACX(41),
000028 1HGX(41)
000029 EQUIVALENCE (ASX, AXS), (ACX, XG), (ASG, AGS), (HXS, HBS), (HXG, HGX), (HSG
000030 1, HGS), (AXG, ACX), (HXG, HGX)
000031 DOUBLE PRECISION C1P, C2P, C3P, D1P
000032 DOUBLE PRECISION C1, C2, D1, D2, P01, PC2, PC3, P1, P2, P3, C3, O, B,
000033 1
000034 DOUBLE C1P, C2P, X, DT
000035 EQUIVALENCE (NDX, NDX1)
000036 C
000037 TIME=60.*TIME
000038 WRITE (6,100) NCYCLE, TIME, TIMEA, DI
000039 WRITE (6,101)
000040 WRITE (6,102) (N,PT(N),TG(N),TS(N),TC(N),TX(N),NS,NDX)
000041 IF( NPSET(1) .GT. 0) OR. (NPSET(2) .GT. 0) GO TO 99
000042 WRITE (6,200)
000043 WRITE (6,201) (N,X(N),PR(1,N),PR(2,N),N=1,NDX)
000044 99 WRITE (6,202)
000045 N1=NDX+1
000046 NDR4=NDR4-1
000047 DO 20 N= 1, NDX
000048 SUMMS=0.
000049 SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000050 IF(NDR4.EQ.2) GO TO 20
000051 DO 22 NR=2, NDR3
000052 22 SUMMS=SUMMS+W(NR,N)
000053 AVLD(N)=SUMMS/NDR3
000054 20 CONTINUE
000055 DO 30 N= N1,NDX1
000056 SUMMS=0.0
000057 SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000058 IF(NDR4.EQ.2) AVLD(N) = SUMMS

```



```

000059 IF(NDR4,EG,2) GO TO 30
000060 DO 33 NR=2, NDR3
000061 33 SUMMS=SUMMS+W(NR,N)
000062 AVLD(N)=SUMMS/NDR3
000063 30 CONTINUE
000064 IF(NDXMAC .EQ. 0) GO TO 35
000065 SUM=0.
000066 DO 31 N= 1, NDXMAC
000067 31 SUM=SUM+AVLD(N)*ABED(N)*DX*HOSB(IN)
000068 AVMSLD = SUM/WTACMS
000069 35 CONTINUE
000070 IF((NDX1-NDXM) .EQ. 0) GO TO 40
000071 SUM=0.
000072 DO 32 N= N1,NOX1
000073 32 SUM =SUM+AVLD(N)*ABED(N)*DX*HOSB(IN)
000074 AVSGLD=SUM/WTSC
000075 40 CONTINUE
000076 DO 10 N=1,NDX
000077 10 WRITE (A,203)N, AVLD(N)
000078 1 WRITE (A,205) AVMSLD, AVSGLD
000079 IF(TIME .LT. 1.E-20) AVMSL1=AVMSLO
000080 IF(TIME .LT. 1.E-20) AVSGL1=AVSGLD
000081 IF(TIME .LT. 1.E-20) AVSGL1=AVSGLD
000082 AVRCO2=WTACMS*(AVMSL1-AVMSLD)/TIME
000083 AVRH2O=WTSC*(AVSGL1-AVSGLD)/TIME
000084 WRITE(6,204) AVRCO2,AVRH2O
000085 RETURN
000086
000087 C
000088 100 FORMAT (1M3,16HDESORPTION CYCLE 13/
000089 1 3M,5HTIME=F9.5,1X2MHR,F12.3,1X,3MMIN,
000090 1 5X,15HTIME INCREMENT=F7.5,1X2MHR)
000091 101 FORMAT (/2X,10MAXIAL NODE,10X,14HTOTAL PRESS,MM,6X,14MGAS TEMP,DE
000092 1 1G,F,5X,19MSORBENT TEMP,DEG F,2X,18HCOOLANT TEMP,DEG F,2X,19HMX CO
000093 2RE TEMP, DEG F )
000094 102 FORMAT(/19,11X,5(F14.4,6X))
000095 103 FORMAT (/21HCO2 DESORPTION RATE=F7,4,1X5HLB/HR,5X,20HH2O DESORPTI
000096 1 10N RATE=F7,4,1X5HLB/HR)
000097 200 FORMAT (1H0/2X,10MAXIAL NODE,13X,9HMOLE FRAC,7X,
000098 1 12X,13HCO2 RATE,1M/HR,6X,13HH2O RATE,1M/HR)
000099 201 FORMAT(/(19,11X,5(F12.6,6X))
000100 1E,3X, 3HAVG: 9X)
000101 1 1H1,9X,1H2,9X,1M3, 9X,1M4,9X,1M5, 9X,1H6,9X,1H7, 9X,
000102 21M6, 9X,1H9,6X,2H10,
000103 28X,2H11/6H AXIAL/5H NODE)
000104 203 FORMAT ( 15,4X,12(F6.4,4X))
000105 204 FORMAT(/27HTIME AVG CO2 DESORP RATE =
000106 1 F8.4, 6H LB/HR,10X,
000107 22TH TIME AVG H2O DESORP RATE =
000108 3 F8.4, 7H LB/HR
000109 205 FORMAT(/27JOM AVG CO2 LOADING IN M.S. BED = F8.4,1X,5HLB/LB,7X,
000110 13OH AVG H2O LOADING IN S.G. BED = F8.4, 6H LB/LB)
000111 END

```



• ELT S9991.1.590501. 43601

```

000001 SUBROUTINE HXCORE(TX,TC,TS,TG,HXC,HXS,HYG,RHOX,CPX,TKX,DX,DT,NDX,A
000002 1VX,NDXM)
000003
000004 C
000005 DIMENSION TX(1),TC(1),TS(1),TG(1),HXC(1),HXS(1),HYG(1),RHOX(1),
000006 1CPX(1),TKX(1),AVX(1)
000007 DIMENSION C1(41),C2(41),C3(41),D1(41)
000008 COMMON /BLOK6/ D10,TS1(41),TS2(41),TX1(41),TX2(41),TC1(41),TC2(41)
000009 DN=DT+D10
000010 DO 10 N=1,NDX
000011 T1= AVX(N)*(HXC(N)+HXS(N)+HYG(N))*0.5
000012 C1(N)= -TKX(N)/DX/DX
000013 C2(N)= -RHOX(N)*CPX(N)/DN -C1(N) - C3(N) + T1
000014 10 D1(N) = RHOX(N)*CPX(N)/DN+TX2(N) + AVX(N)*(HXC(N)
000015 1*TC2(N) + HXS(N)*TS1(N)+HYG(N)*TG(N)) - T1*TX2(N)
000016 C2(1)=C2(1)+C1(1)
000017 C1(1)=0.
000018 C2(NDX)=C2(NDX)+C3(NDX)
000019 C3(NDX)=0.0
000020 CALL FDEG1M(C1,C2,C3,D1,TV,NDX)
000021 RETURN
000022 END

```



• ELT S9996.1.690501. 13802

```

000001 SUBROUTINE LAGIN2(ID,X,NP,ND,XD,YO,Y)
000002 REVISD FOR FORTRAN IV 8-8-65 S. WONG
000003 DIMENSION X(2), Y(2)
000004
000005 ILO=1
000006 IF(XO-X(1))10,16,4
000007 4 IF(XO-X(NP))19,13,7
000008 7 ILO=NP-1
000009 10 IMI=ILO+1
000010 WRITE (6,1) ID,XO
000011 GO TO 46
000012 13 ILO=NP
000013 16 YOR(ILO)
000014 RETURN
000015 19 DO 22 ILO=2,NP
000016 IF(XO-X(ILO))25,16,22
000017 22 CONTINUE
000018 25 IMI=ILO
000019 ILO=IMI-1
000020 IF(ND-2)46,46,28
000021 28 DO 43 I=3,ND
000022 IF(ILO-1)40,40,31
000023 31 IF(IMI=NP)34,37,39
000024 34 IF (2.*XO-X(ILO-1)-X(IMI+1)) 37,37,40
000025 37 ILO=ILO-1
000026 GO TO 43
000027 40 IMI=IMI+1
000028 43 CONTINUE
000029 46 YOR(I)
000030 PN=1.0
000031 DO 48 I=ILO,IMI
000032 PN=PN*(XO-X(I))
000033 DO 58 I=ILO,IMI
000034 P=PN/(XO-X(I))
000035 DO 55 J=ILO,IMI
000036 IF(J-I)52,55,52
000037 52 P=Z/(X(I)-X(J))
000038 55 CONTINUE
000039 YOR(YO+P*Y(I))
000040 58 CONTINUE
000041 RETURN
000042 1 FORMAT (9X,7HLAGIN2 ,14,E12.5)
000043 END

```



9-ELT-9997.1-690501-43804

```

000001 SUBROUTINE ISORB
000002 COMMON /BLOK1/ ABED(41), A(41), AVC(41), CPG(41), RHOG(41),
000003 IHG(41), HXS(41), HXC(41), DIF(41), F(41), C(41), VS(2), DVS(2), DVS1(2), R
000004 2S1(2,41), RHOS(2), UC(41), WM(2), UC(41), NDXM, PS(41), RHOSB(41), DS(41),
000005 3CS1(41), CS2(41), C1(21,41), C2(21,41), D1(21,41), D2(41), PC1(41), PC2(4
000006 41), PC3(41), ASG(41), ASX(41), ACX(41), C1P(41), C2P(41), C3P(41), D1P(41)
000007 5, BR(2,41), RS(2), NOX1, NDM4, DM, DT, CK(41), DM(41), SK(41), P1(41), P2(41)
000008 6, P3(41), WS(41), CR1(2,21), CR2(2,21), CR3(2,21), C3(21,41), B(21,41),
000009 7Q(21,41), CR1(41), CP2(41), X(41), VOIDE(41), TIME
000010 8, AX(41), RHOC(41), CPC(41), Y88, AVX(41), TXK(41), CPX(41), RHOX(41)
000011 9, NOG, PK(2,41), PCO21, PW201, CWR, CW, TGL, PA, PT(41), CRS(41), WSG(41)
000012 DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, P1, P2, P3, C3, O, B,
000013 1 CPI, CP2, X, DT
000014 DOUBLE PRECISION C1P, C2P, C3P, D1P
000015 COMMON /BLOK3/ M(21,41), TG(41), TS(41), TX(41), TC(41), TX1(41), TC2(41)
000016 DOUBLE PRECISION V
000017 COMMON /BLOK8/ DTO, T64(41), TS2(41), TX1(41), TX2(41), TC1(41), TC2(41)
000018 DIMENSION S1(41), S2(41), S3(41), B1(41)
000019 DO 10 N=1, NDX1
000020 T=(DT+DT0)/CPI(N)/RHOSB(N)
000021 I=90.5*E/(ASG(N)+WSG(N)+ASX(N)+HXS(N))
000022 C81(N)=C81(N)*(1.0+T)
000023 C82(N)=C82(N)*(1.0+T)
000024 B1(N)=T*S2(N)+C81(N)+C82(N)-C82(N)*(P1(N)+P2(N))*(N+NDRA,N)-WS(N))*
000025 1 P1(N)+P1(N)+T*(ASG(N)+WSG(N)+ASX(N)+HXS(N))
000026 2 IF(N.EQ.1) S1(N)=0
000027 IF(N.EQ.1) GO TO 11
000028 S1(N)=T*8K(N)/DX/DM*(ABED(N-1)+ABED(N))/(2.*ABED(N))
000029 S1(N)=T*8K(N)/DX/DM*(ABED(N-1)+ABED(N))/(2.*ABED(N))
000030 S1(N)=T*8K(N)/DX/DM*(ABED(N)+ABED(N+1))/(2.*ABED(N))
000031 S2(N)=S1(N)-S1(N)-S3(N)+T
000032 10 CONTINUE
000033 CALL FDEQ(MIS1, S2, S3, B1, T6, NDX1)
000034 RETURN
000035 END

```

END CUR UCC 174



PART II

MULTIPLE BED PROGRAM (MAIN4B)



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NOMENCLATURE

<u>FORTTRAN</u>	<u>Algebraic*</u>	<u>Description</u>
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)
AVH20P		Average poisoning rate of molecular sieves by H ₂ O, (lb-H ₂ O)/hr
AVMSLD		Average CO ₂ -loading of all active molecular sieve sorbents, lb-CO ₂ /(lb-molecular sieves)
AVPH20		Average outlet P _{H₂O} , mm Hg
AVRC02		Average CO ₂ adsorption or desorption rate, lb-CO ₂ /hr
AVRH20		Average H ₂ O adsorption or desorption rate, lb-H ₂ O/hr
AVSGLD		Average H ₂ O-loading of desiccant sorbents, lb-H ₂ O/(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.



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
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/(°F)(lb)
CPG	C_{pg}	Heat capacity of gas mixture, Btu/(°F)(lb)
CPL		Specific heat of adsorbed sorbate, Btu/(°F)(lb)
CPP		Specific heat of dry sorbent, Btu/(°F)(lb)
CPS	C_{ps}	Sorbent specific heat, Btu/(lb)(°F)
CPX	C_{px}	Heat capacity of heat exchanger metal, Btu/(°F)(lb)
CPI	}	Coefficients in equation
CP2		$PC3 \cdot (P_{ks,t + \Delta t}) - X_k P_{t + \Delta t} = CPI + CP2 \cdot P_{t + \Delta t}$
CR1	}	Coefficients in following equation which is merely another form of Equation (2-28), in Part I of this report.
CR2		
CR3		$CR1 \cdot \frac{W_{k,M,(t + \Delta t)} - W_{k,M,t}}{(\Delta t)} = CR2 \cdot (W_{k,(M-1)}(t + \Delta t) - W_{k,M,(t + \Delta t)} + CR3 \cdot (W_{k,M,(t + \Delta t)} - W_{k,(M+1)}(t + \Delta t))$
CS1	}	Coefficients in equation
CS2		$T_s(t + \Delta t) - T_{s,t} = DS + CS1 \cdot P(t + \Delta t) - CS2 \cdot P_{ks,(t + \Delta t)}$
CYCLE		Cycle time per one adsorption or one desorption half-cycle, hr
CI	}	Coefficients in equation
C2		$C1 \cdot W(t + \Delta t), (M-1) + C2 \cdot W(t + \Delta t), M$
C3		$+ C3 \cdot W(t + \Delta t), (M + 1) = DI$



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
C1P	}	Coefficients in equation
C2P		$C1P \cdot P(t + \Delta t), (N-1) + C2P \cdot P(t + \Delta t), N$
C3P		$+ C3P \cdot P(t + \Delta t), (N + 1) = DIP$
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 CSI
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
DI		See CI
DIP		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 ₂ O, during desorption, FR (1,N) is CO ₂ rate, FR (2,N) is H ₂ O rate, lb-mole/hr



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
	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
HGX, HXC	h_{xc}	Heat transfer coefficient between heat exchanger primary plate and coolant, Btu/(sq ft)(°F)(hr)
HGS, HSG	h_{sg}	Heat transfer coefficient between sorbent and gas, based on a_{sg} , Btu/(sq ft)(°F)(hr)
HXS, HXS	h_{xs}	Effective heat transfer coefficient between heat exchanger primary plate and sorbent, Btu/(sq ft)(°F)(hr)
HTR		Same as HTRI if $IST\emptyset PC = 0$. This variable is used in program
HTRI		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)(°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



<u>FORTTRAN:</u>	<u>Algebraic</u>	<u>Description</u>
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 \neq 0, WC = 0, HTR = 0, SABCO2 = 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 nodes, 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



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
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



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
PC1		Coefficients in equation for desorption pressure
PC2	$\left. \begin{aligned} & \frac{P(t+\Delta t), N - P_t, N}{(\Delta t)} \\ & = PC1 \cdot \frac{P(t+\Delta t), N-1 - 2P(t+\Delta t), N + P(t+\Delta t), (N-1)}{(\Delta x)^2} \\ & + PC2 \cdot \frac{P(t+\Delta t), (N+1) - P(t+\Delta t), (N-1)}{2(\Delta x)} \\ & + PC3 \cdot [P_{ks}(t+\Delta t) - X_k P(t+\Delta t)] \end{aligned} \right\}$	
PC3		
PH20C		H ₂ O partial pressure in the cabin, mm Hg
PH20I		Inlet H ₂ O partial pressure, mm Hg
PH20I1	$\left. \begin{aligned} & PH20I \text{ for bed 1, 2, 3 and 4, respectively} \end{aligned} \right\}$	
PH20I2		
PH20I3		
PH20I4		
PK(K,N)	P_k	$p \cdot X_k$; partial pressure of component k in bulk gas stream, mm Hg
PK1	$\left. \begin{aligned} & PK \text{ for bed 1, 2, 3 and 4, respectively} \end{aligned} \right\}$	
PK2		
PK3		
PK4		
PN2		N ₂ partial pressure for overboard loss computation
PN21	$\left. \begin{aligned} & PN2 \text{ for bed 1, 2, 3 and 4, respectively} \end{aligned} \right\}$	
PN22		
PN23		
PN24		
P0UT		10 tabulated desorption outlet pressures at TIMET, mm Hg
P02		O ₂ partial pressure for overboard loss calculations
P021	$\left. \begin{aligned} & P0_2 \text{ for bed 1, 2, 3, and 4, respectively} \end{aligned} \right\}$	
P022		
P023		
P024		
PS		Variable for a temporary storage of PT



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
PT	P	Total pressure in bulk gas stream, mm Hg
PT1	}	PT for bed 1, 2, 3 and 4, respectively
PT2		
PT3		
PT4		
PUMP		Pressure ratios at which vacuum pump displacements VPUMP are tabulated
PI	}	Coefficients in equation
P2		
P3		
		$P_{ks}(t+\Delta t) = P1 + P2 \cdot (W_{k,s}(t+\Delta t) - W_{k,s,t}) + P3 \cdot P$
Q		Temporary variable like B. See Equations (2-43) and (2-44), 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)(°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)



<u>FORTRAN</u>	<u>Algebraic</u>	<u>Description</u>
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 $\int_{t=zero}^t P_{H_2O, outlet} \cdot (\Delta t)$, (mm)(hr)
TC	T_c	Coolant temperature, °F
TCØ2A		CO ₂ -accumulator temperature, °F
TCIN		Identical with T268, inlet coolant temperature, °F
TCØ1 TCØ2 TCØ3 TCØ4		} Initial TC for bed 1, 2, 3 and 4, respectively
TCI		Coolant temperature at time, $t - \Delta t$
TCI1 TCI2 TCI3 TCI4		} TCI for bed 1, 2, 3, and 4, respectively



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
TC2		Coolant temperature at time, $t - 2\Delta t$
TC21	}	TC2 for bed 1, 2, 3 and 4, respectively
TC22		
TC23		
TC24		
TG	T_g	Gas temperature, $^{\circ}\text{F}$
TGC		Cabin temperature, $^{\circ}\text{F}$
TGHX		Maximum allowable temperature at molecular sieve bed inlet, above which an intercooler will be used to lower it to TGHX, $^{\circ}\text{F}$
TGI	T_{gi}	Inlet gas temperature for adsorption cycle, $^{\circ}\text{F}$
TGI1	}	TGI for bed 1, 2, 3, and 4, respectively
TGI2		
TGI3		
TGI4		
TG1	}	TG for bed 1, 2, 3, and 4, respectively
TG2		
TG3		
TG4		
TI		Maximum temperature change allowable per time increment in selecting Δt , $^{\circ}\text{F}$
TIME	t	Time from beginning of each adsorption 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) ($^{\circ}\text{F}/\text{ft}$)
TMAX		Maximum allowable sorbent temperature, above which heater will be shut off, $^{\circ}\text{F}$
TØTCØ2		Total amount of CO_2 adsorbed since beginning of adsorption period, lb



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



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
T268	T_{268}	Inlet coolant temperature, °F
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 sieve sorbents, lb
WTMS		Total weight of molecular sieve sorbents, lb
WTSG		Total weight of desiccants, lb
W1	}	W for bed 1, 2, 3 and 4, respectively
W2		
W3		
W4		



<u>FORTTRAN</u>	<u>Algebraic</u>	<u>Description</u>
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 ₂ O 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
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 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

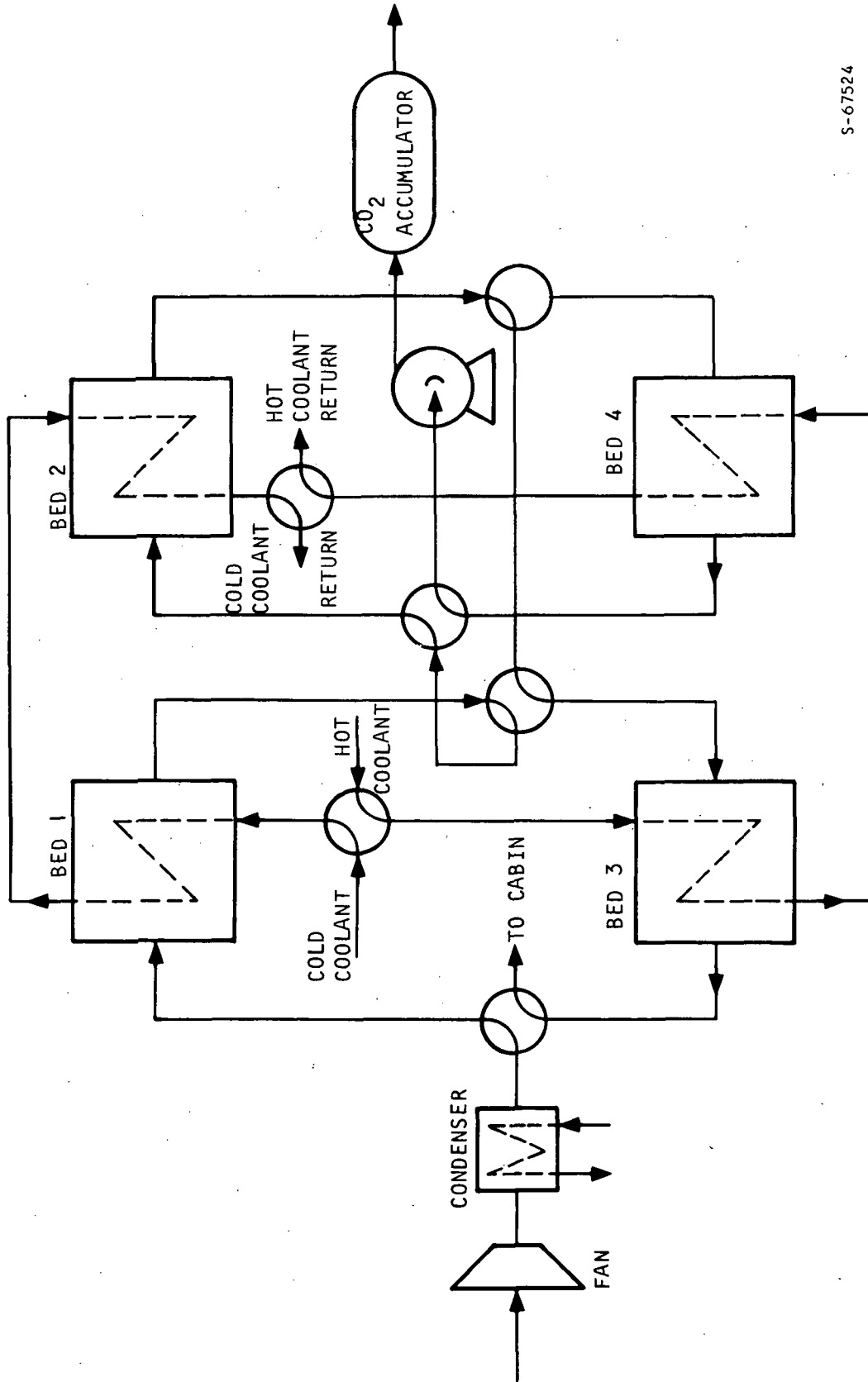
The input to MAIN4B is by means of eleven namelists. The lists include initial conditions, bed sizes, mass and heat transfer coefficients, etc. However, equilibrium data of various sorbate-sorbent pairs are all contained in subroutines EQPWT and FC0AD in the form of data statements. These may have to 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





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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) CO₂-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-H₂O-save-CO₂-dump
- (c) 4-bed-H₂O-CO₂-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 CO₂ accumulator pressure.
- (i) Use of a constant pressure type CO₂-accumulator
- (j) Use of a constant volume type CO₂-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

$$S = \frac{S_p C}{S_p + C} \quad (7-1)$$

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

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

where P_{av} = average duct pressure, torrs

D = duct diameter, cm

L = duct length, cm

M = molecular weight

T = temperature, °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 DESORB can also be changed for different configurations.

PUMPING INTO A CO₂-ACCUMULATOR

For a CO₂-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

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

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

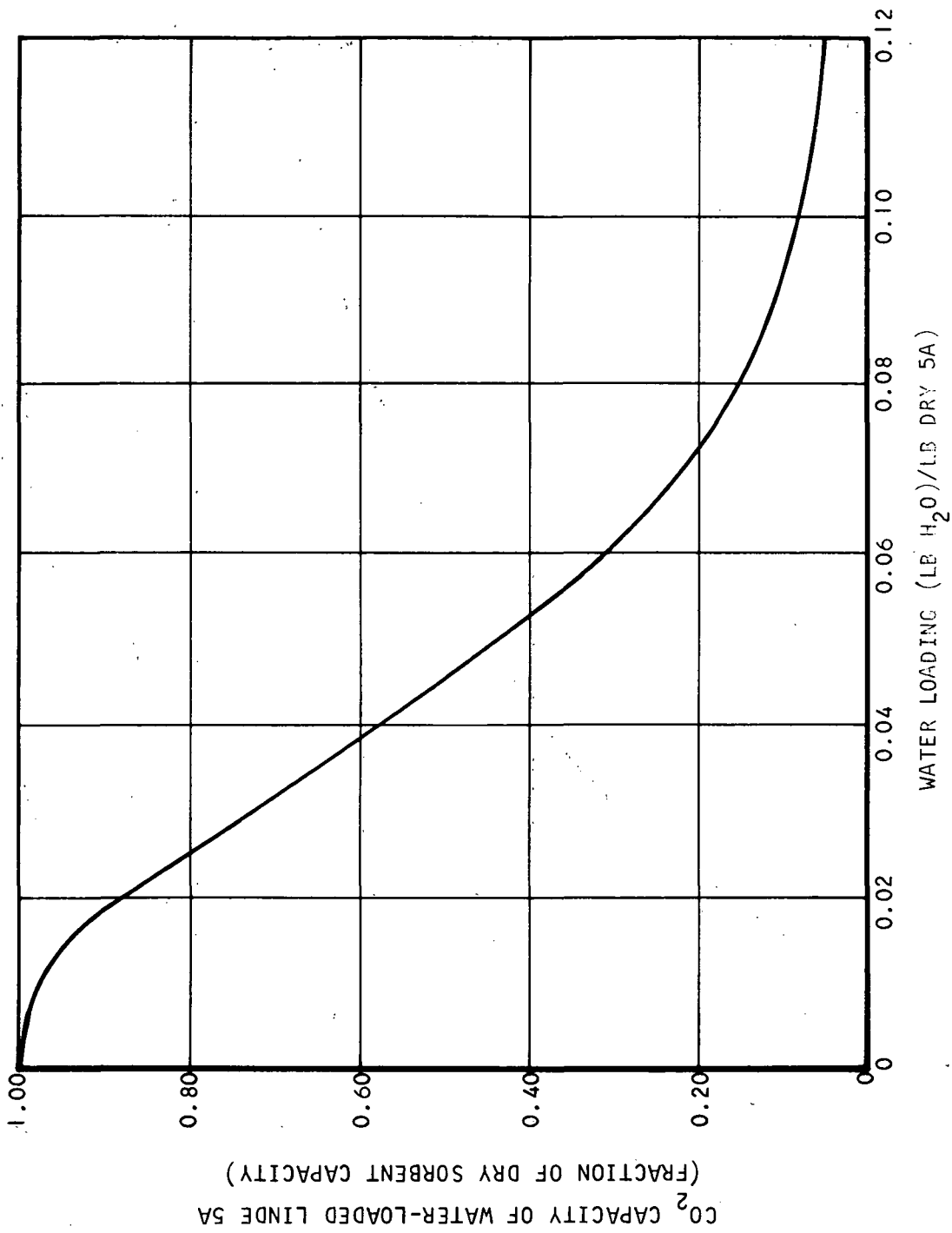
$$\left(c_{px} \cdot \rho_x \right) \frac{\partial T_x}{\partial t} = \frac{\partial}{\partial x} \left(k_x \frac{\partial T_x}{\partial x} \right) + a_{vx} \cdot \left[h_{xs} (T_s - T_x) + h_{xg} (T_g - T_x) + h_{xc} (T_c - T_x) \right] + \dot{Q}_v \quad (7-4)$$

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 FC0AD, in the form of H₂O loading vs CO₂ 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.

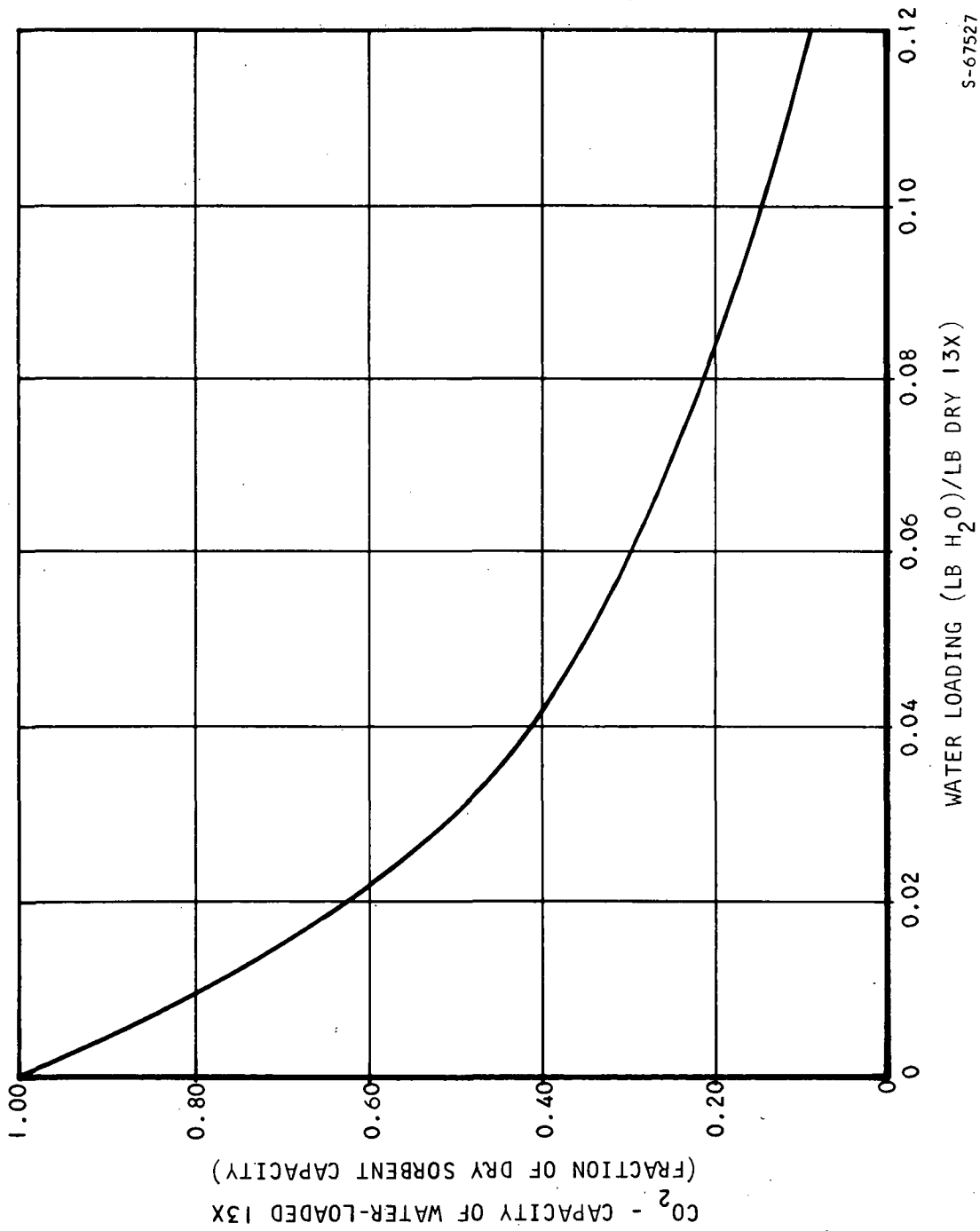




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Figure 7-1. Effect of Water Poisoning on Linde 5A Capacity for CO₂





S-67527

Figure 7-2. Effect of Water Poisoning on Linde 13X Capacity for CO₂



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.

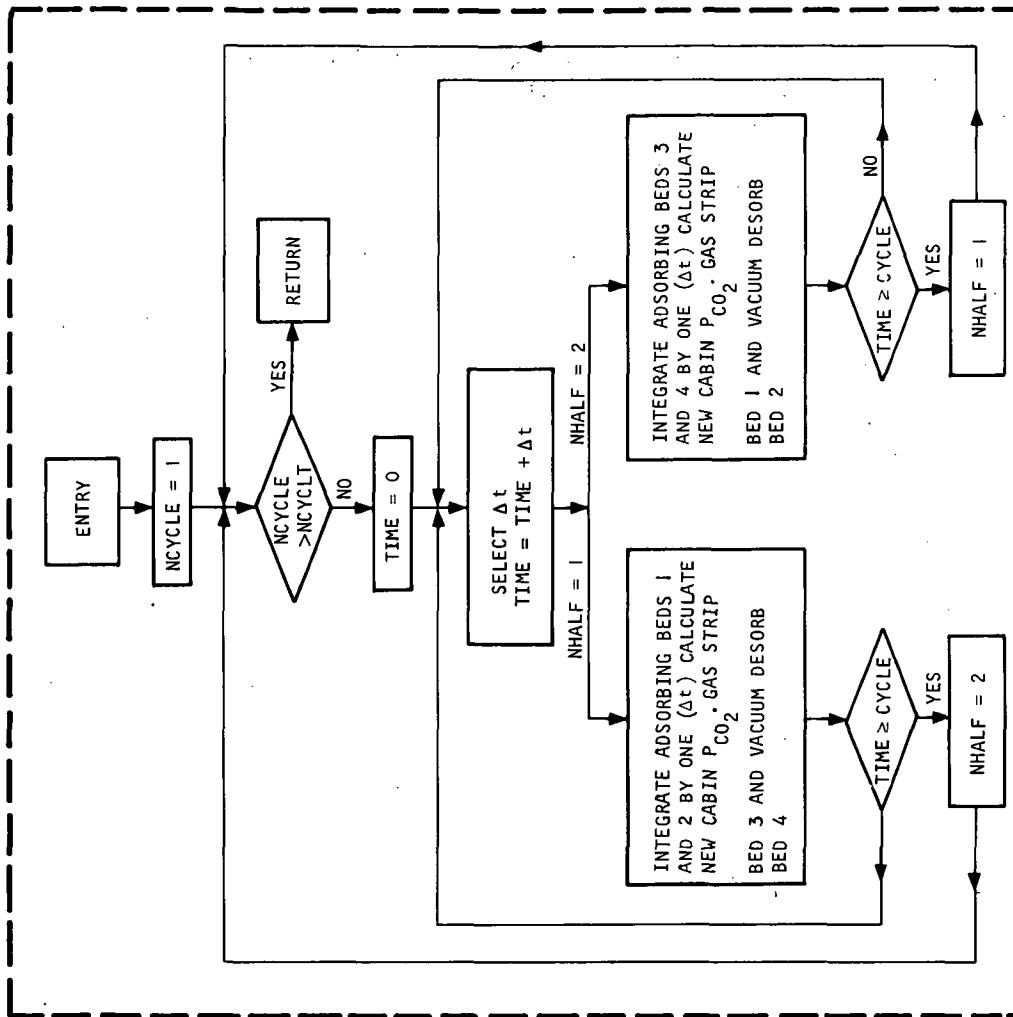
In the input data, NDXM and NDXMAC for each bed are selected so that the CO_2 sorbent nodes which may potentially be poisoned in NCT1 cycles are assigned as desiccant nodes. This results in a desiccant section greater, and a CO_2 -sorbent section smaller, than the actual sizes. The program is run for 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.

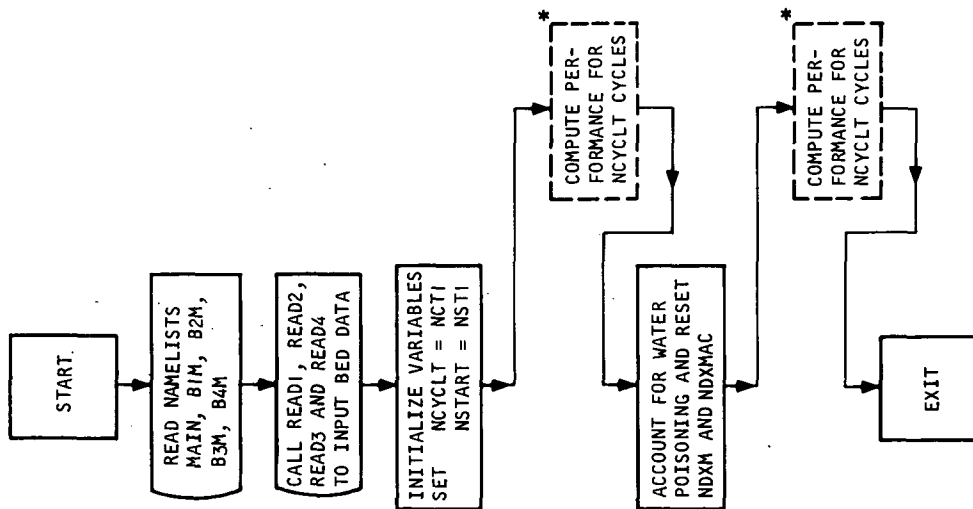
In Figure 7-3, the 4-bed performance prediction is performed by the operations enclosed in the broken-line rectangle, which are shown in the right hand portion of the figure.





S-67595

Figure 7-3. MAIN4B Program Logic



*OPERATIONS ENCLOSED BY BROKEN LINES EXPANDED IN BLOCK AT RIGHT



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, CO₂-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 Definition1. Namelist MAIN

<u>Fortran Symbol</u>	<u>Definition</u>
WM(2)	Adsorbate molecular weight; eg., WM(1) = (CO ₂), WM(2) = 18 (H ₂ O)
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 , $^{\circ}\text{F}$
PC \emptyset 2C	Initial CO_2 partial pressure in cabin, mm Hg
V \emptyset LCAB	Cabin volume for atmosphere, cu ft; use $V\emptyset\text{LCAB} = 10^{20}$, for constant PC \emptyset 2C
RC \emptyset 2C	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
NDTC \emptyset N	If NDTC \emptyset N = 1, Δt will be selected such that $\Delta T = \text{TI}$, $\Delta W = \text{WI}$ for time step; if NDTC \emptyset N = 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, $^{\circ}\text{F}$
PAC	Cabin pressure, mm Hg
PH $2\emptyset$ C	Cabin $P_{\text{H}_2\text{O}}$, 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.
PC \emptyset 2A	CO_2 accumulator pressure, for a fixed volume type, psia
VC \emptyset 2A	CO_2 accumulator volume for a fixed pressure type, cu ft
SABC \emptyset 2	CO_2 flow-rate to Sabatier reactor, lb CO_2 /hr.
TC \emptyset 2A	CO_2 accumulator temperature, $^{\circ}\text{F}$



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-desorp- tion cycle calculations desired before effects of bed-poisoning will be assessed and bed sized adjusted accordingly to pre- dict 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 BIM

<u>Fortran Symbol</u>	<u>Definition</u>
PAI	Bed No. 1 total pressure, mm Hg
TSO1(20)	Bed No. 1 initial sorbent temperature, °F
TCO1(20)	Bed No. 1 initial coolant temperature, °F
TXO1(20)	Bed No. 1 initial HX metal temperature, °F
WI (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

<u>Fortran Symbol</u>	<u>Definition</u>
PA2	Bed No. 2 total pressure, mm Hg
TS02(20)	Bed No. 2 initial sorbent temperature, °F
TC02(20)	Bed No. 2 initial coolant temperature, °F
TX02(20)	Bed No. 2 initial HX metal temperature, °F
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

<u>Fortran Symbol</u>	<u>Definition</u>
PA3	Bed No. 3 total pressure, mm Hg
TS03	Bed No. 3 initial sorbent temperature, °F
TC03	Bed No. 3 initial coolant temperature, °F
TX03	Bed No. 3 initial HX metal temperature, °F
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

<u>Fortran Symbol</u>	<u>Definition</u>
PA4	Bed No. 4 adsorption cycle total pressure, mm Hg
TS04	Bed No. 4 initial sorbent temperature, °F
TC04	Bed No. 4 initial coolant temperature, °F
TX04	Bed No. 4 initial HX metal temperature, °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

<u>Fortran Symbol</u>	<u>Definition</u>
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)(°F)
CPC (20)	Coolant specific heat, Btu/(lb)(°F)
CPX (20)	Heat exchanger specific heat, Btu/(°F)(lb)
CPP (20)	Specific heat of dry sorbent, Btu/(lb)(°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)	} 10 pairs of exit pressure vs time data to be used if NBCOUT = 2; PØUT = vacuum end manifold pressures (mm Hg), TIMET = times (hr)
TIMET (10)	



PUMP (10) VPUMP (10)	} 10 pairs of pressure ratios vs volumetric displacements to be used for NBCOUT = 3 or 4; PUMP = pump outlet to pump inlet pressure ratio; VPUMP = volumetric displacements, cfm.
IDSORB (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/(^o F) (lb)
DP (20)	Sorbent diameter, ft.

7. Namelist DBA

<u>Fortran Symbol</u>	<u>Definition</u>
HXG (20)	Heat transfer coefficient, heat exchanger to process gas, Btu/(sq ft) (^o F) (hr)
HXS (20)	Heat transfer coefficient, heat exchanger to sorbent, Btu/(sq ft)(hr)(^o F)
HXC (20)	Heat transfer coefficient, heat exchanger to coolant Btu/(sq ft)(hr)(^o F)
HSG (20)	Heat transfer coefficient, sorbent to gas, Btu/(hr)(sq ft)(^o F)
SK (20)	Effective sorbent thermal conductivity, Btu/(hr) (sq ft) (^o F/ft)
TKX (20)	Heat exchanger metal thermal conductivity, TKX (K) denotes that between node K-1 and node K, Btu/(hr)(sq ft)(^o 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, ^o F
HTR (20)	Electric heater power for each node, BTU/hr



TMAX Maximum metal temperature, above which heater will be shutt off, °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 CO₂ 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 CO₂ 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 CO₂ 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-CO₂-H₂O-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 N₂ and pure O₂ data are employed by the program in estimating overboard gas losses. Should expanded N₂ - O₂ 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- $\text{CO}_2\text{-H}_2\text{O}$ 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°F .

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, P021, PN22, P022, 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 $\text{NCT1}=6$ and $\text{NST1}=6$ 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 $\text{NCT2}=0$ for the run, the program stops at this point.



		.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,
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,
HSG	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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SK	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.99999998-01,	.00000000+00,	.00000000+00,	.00000000+00,
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TKX	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.90000000+01,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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DH	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
DIF	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.40000000-03,	.40000000-03,	.40000000-03,	.40000000-03,
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GK	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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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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TCIN	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
HTR1	"	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.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,	.00000000+00,	.00000000+00,	.00000000+00,
WCC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
\$END					
\$DBD					
HXG	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.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)

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,	.00000000+00,	.00000000+00,
TIMET	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
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		.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,	.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,	.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,
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\$END					
\$MBA					
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HXS	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.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,
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		.50000000+01,	.50000000+01,	.00000000+00,	.00000000+00,
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		.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,

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,
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		.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,
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		.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,	.20000000-03,	.20000000-03,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TCIN	=	.00000000+00,	.00000000+00,	.00000000+00,	.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,
TMAX	=	.40000000+03,	.40000000+03,	.40000000+03,	.40000000+03,
WCC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
\$END					
\$NBD					
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,	.00000000+00,	.00000000+00,	.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,	.40000000+03,	.40000000+03,	.40000000+03,
WCC	=	.00000000+00,	.00000000+00,	.00000000+00,	.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	PH2O,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

SORB AXIAL 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)	AVG H2O LOADING IN DESICCANT (LB/LB)
.0000	.0806
TIME AVG CO2 ADSORPTION RATE (LB/HR)	TIME AVG H2O ADSORPTION RATE (LB/HR)
.0000	.2592
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)	HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)
.0000	.0000
TIME AVG OUTLET PH2O (MM)	
.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	2.0598	.0000	52.4302	52.5273	-.0000	52.6288
5	2.4923	.0000	50.6066	50.6391	.0000	50.7356
INLET	2.5782	.0000	50.0000			

LOADING AT INTERIOR OF SORBENT, LB/LB

SORB 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)	AVG H2O LOADING IN DESICCANT (LB/LB)
0.0332	0.0000
0.5501	0.0000
0.0000	0.0000
0.0000	0.0000
0.0000	0.0000

TIME AVG CO2 ADSORPTION RATE (LB/HR)
 ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)
 TIME AVG OUTLET PH2O (MM)

TIME AVG H2O ADSORPTION RATE (LB/HR)
 HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)



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 AXIAL NODE	AVG	1	2	3	4
1	.0263	.0263	.0263	.0263	.0263
2	.0329	.0329	.0329	.0329	.0329
3	.0375	.0375	.0375	.0375	.0375
4	.0624	.0624	.0624	.0624	.0624
5	.1114	.1114	.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) .0000

AVG H2O LOADING IN DESICCANT (LB/LB) .9541
 TIME AVG H2O ADSORPTION RATE (LB/HR) .0000
 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 MR

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	389.9976	.0000	389.1141

LOADING AT INTERIOR OF SORBENT

SORB NODE	AVG	1	2	3	4
AXIAL NODE					
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)	AVG H2O LOADING IN DESICCANT (LB/LB)
.0094	.0000
TIME AVG CO2 DESORPTION RATE (LB/HR)	TIME AVG H2O ADSORPTION RATE (LB/HR)
.5505	.0000
ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)	HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)
2.1730	.0000
ACCUMULATOR CO2 PRESSURE (PSIA)	CO2 ACCUMULATOR VOLUME (CU FT)
25.0000	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.



		.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,			
SEND					
\$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,	.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,
		.39999999-01,	.39999999-01,	.39999999-01,	.39999999-01,
		.39999999-01,	.39999999-01,	.39999999-01,	.39999999-01,
		.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
		.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
		.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
		.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
		.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
		.49999999-01,	.49999999-01,	.49999999-01,	.49999999-01,
		.69999998-01,	.69999998-01,	.69999998-01,	.69999998-01,
		.20000000+00,	.20000000+00,	.20000000+00,	.20000000+00,
		.20000000+00,	.20000000+00,	.20000000+00,	.20000000+00,
		.56999999-01,	.56999999-01,	.56999999-01,	.56999999-01,
		.56999999-01,	.56999999-01,	.56999999-01,	.56999999-01,
GMR2	=	.15500000+02,			
GMW2	=	.31000000+02,			
PN22	=	.65000000+02,			
PO22	=	.19300000+03,			
SEND					
\$B3M					
PA3	=	.00000000+00,			
TS03	=	.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
		.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
		.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
		.45000000+02,	.45000000+02,	.45000000+02,	.45000000+02,
		.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)



		.96000000+01,	.96000000+01,	.96000000+01,	.96000000+01,
		.96000000+01,	.96000000+01,	.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	=	.99999998-01,	.99999998-01,	.99999998-01,	.99999998-01,
		.99999998-01,	.99999998-01,	.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,
TKX	=	.90000000+01,	.90000000+01,	.90000000+01,	.90000000+01,
		.90000000+01,	.90000000+01,	.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,
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	=	.40000000-04,	.40000000-04,	.40000000-04,	.40000000-04,
		.40000000-04,	.40000000-04,	.40000000-04,	.40000000-04,
		.40000000-04,	.40000000-04,	.40000000-04,	.40000000-04,
		.40000000-04,	.40000000-04,	.40000000-04,	.40000000-04,
GK	=	.49999999-02,	.49999999-02,	.49999999-02,	.49999999-02,
		.49999999-02,	.49999999-02,	.49999999-02,	.49999999-02,
		.49999999-02,	.49999999-02,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
		.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
TCIN	=	.00000000+00,	.00000000+00,	.00000000+00,	.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,
TMAX	=	.40000000+03,	.40000000+03,	.40000000+03,	.40000000+03,
WCC	=	.00000000+00,	.00000000+00,	.00000000+00,	.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)

		.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,
		.40000000+03,	.40000000+03,	.40000000+03,	.40000000+03,
		.40000000+03,	.40000000+03,	.40000000+03,	.40000000+03,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
DIF	=	.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
GK	=	.49999999-03,	.49999999-03,	.49999999-03,	.49999999-03,
		.49999999-03,	.49999999-03,	.49999999-03,	.49999999-03,
		.49999999-03,	.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,	.00000000+00,	.00000000+00,	.00000000+00,
HTK1	=	.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,	.40000000+03,	.40000000+03,	.40000000+03,
WCC	=	.00000000+00,	.00000000+00,	.00000000+00,	.00000000+00,
\$END					
\$MBD					
HXG	=	.15100000-01,	.15100000-01,	.15100000-01,	.15100000-01,
		.15100000-01,	.15100000-01,	.15100000-01,	.15100000-01,
		.15100000-01,	.15100000-01,	.15100000-01,	.15100000-01,
		.15100000-01,	.15100000-01,	.15100000-01,	.15100000-01,
		.15100000-01,	.15100000-01,	.00000000+00,	.00000000+00,
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,
		.55000000+00,	.55000000+00,	.55000000+00,	.55000000+00,
		.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,
		.11600000+02,	.58000000+01,	.79999998-01,	.79999998-01,
		.79999998-01,	.79999998-01,	.79999998-01,	.79999998-01,
		.79999998-01,	.79999998-01,	.00000000+00,	.00000000+00,
TKX	=	.00000000+00,	.90000000+01,	.90000000+01,	.90000000+01,
		.90000000+01,	.90000000+01,	.90000000+01,	.90000000+01,
		.90000000+01,	.90000000+01,	.90000000+01,	.90000000+01,
		.90000000+01,	.90000000+01,	.90000000+01,	.90000000+01,
		.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,
		.40000000+03,	.40000000+03,	.40000000+03,	.40000000+03,
		.40000000+03,	.40000000+03,	.40000000+03,	.14000000+04,

Figure 9-4. (Continued)



		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
		.14000000+04,	.14000000+04,	.14000000+04,	.14000000+04,
DTF	=	.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
		.99999998-04,	.99999998-04,	.99999998-04,	.99999998-04,
GK	=	.49999999-03,	.49999999-03,	.49999999-03,	.49999999-03,
		.49999999-03,	.49999999-03,	.49999999-03,	.49999999-03,
		.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,	.00000000+00,	.00000000+00,	.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,
TMAX	=	.40000000+03,	.40000000+03,	.40000000+03,	.40000000+03,
WCC	=	.00000000+00,	.00000000+00,	.00000000+00,	.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	WX CORE TEMP, F
1	2.4117	.0360	71.5705	71.5572	69.9997	70.5092
2	2.6671	.0380	72.6753	72.6678	69.9997	70.9539
3	2.9419	.0360	73.3119	73.3130	69.9997	71.7848
4	3.2348	.0360	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	108.9593	69.9997	71.5795
16	5.3367	7.5879	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

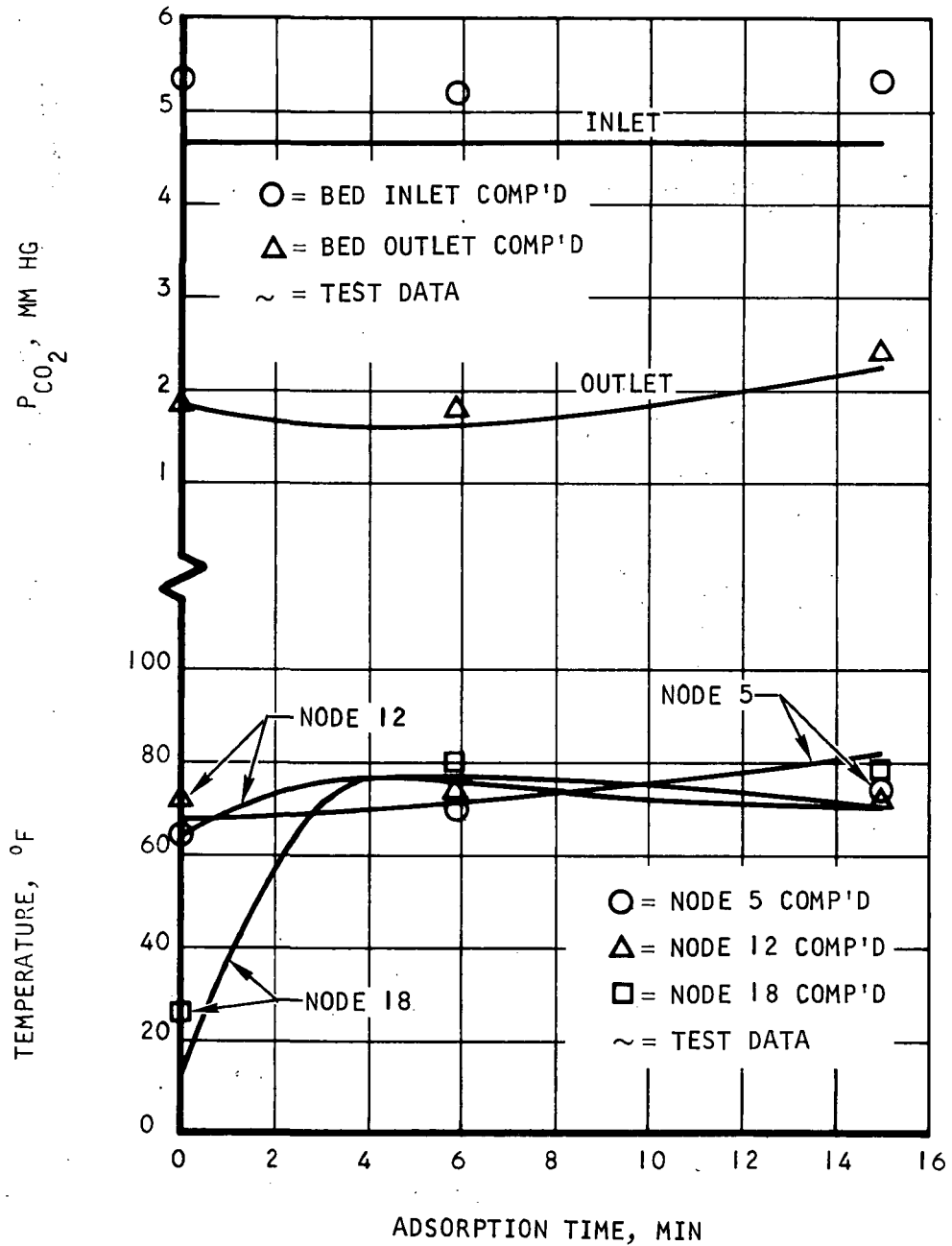
SORB AXIAL NODE	1	2	3	4
1	.0334	.0331	.0336	
2	.0346	.0343	.0349	
3	.0361	.0358	.0364	
4	.0381	.0378	.0385	
5	.0398	.0394	.0402	
6	.0416	.0412	.0420	
7	.0435	.0431	.0440	
8	.0456	.0452	.0460	
9	.0477	.0473	.0481	
10	.0498	.0494	.0502	
11	.0525	.0522	.0528	
12	.0929	.0928	.0928	
13	.1563	.1502	.1568	
14	.1744	.1724	.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
 TIME AVG CO2 ADSORPTION RATE (LB/HR) .2609
 AVG H2O LOADING IN DESICCANT (LB/LB) .1849
 TIME AVG H2O ADSORPTION RATE (LB/HR) .3480

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

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





S-70266

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

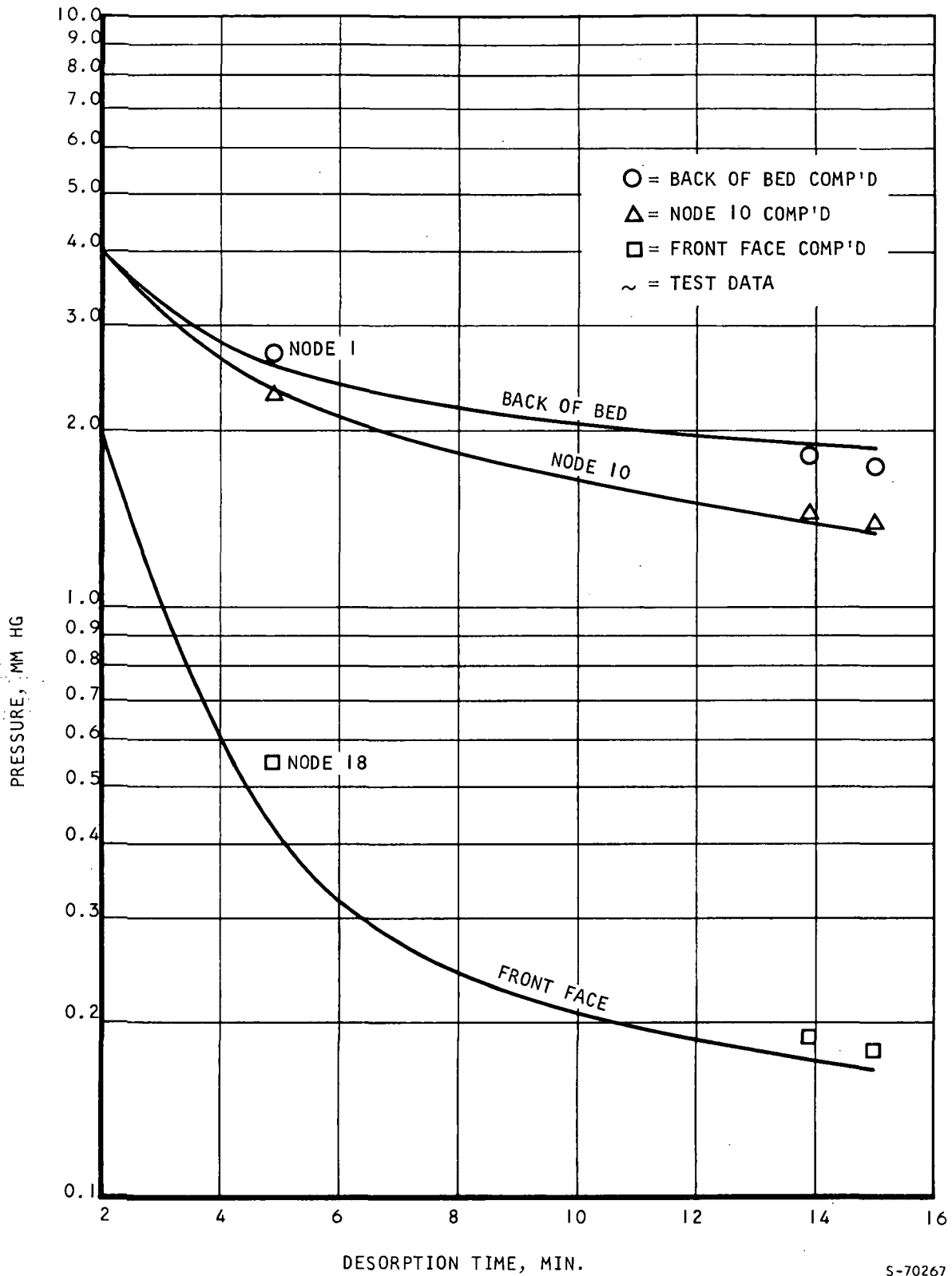


Figure 9-10. Comparison of Computed Desorption Pressures with Test Data (Cycle 94 of 28 Day Test)



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 CO₂-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:

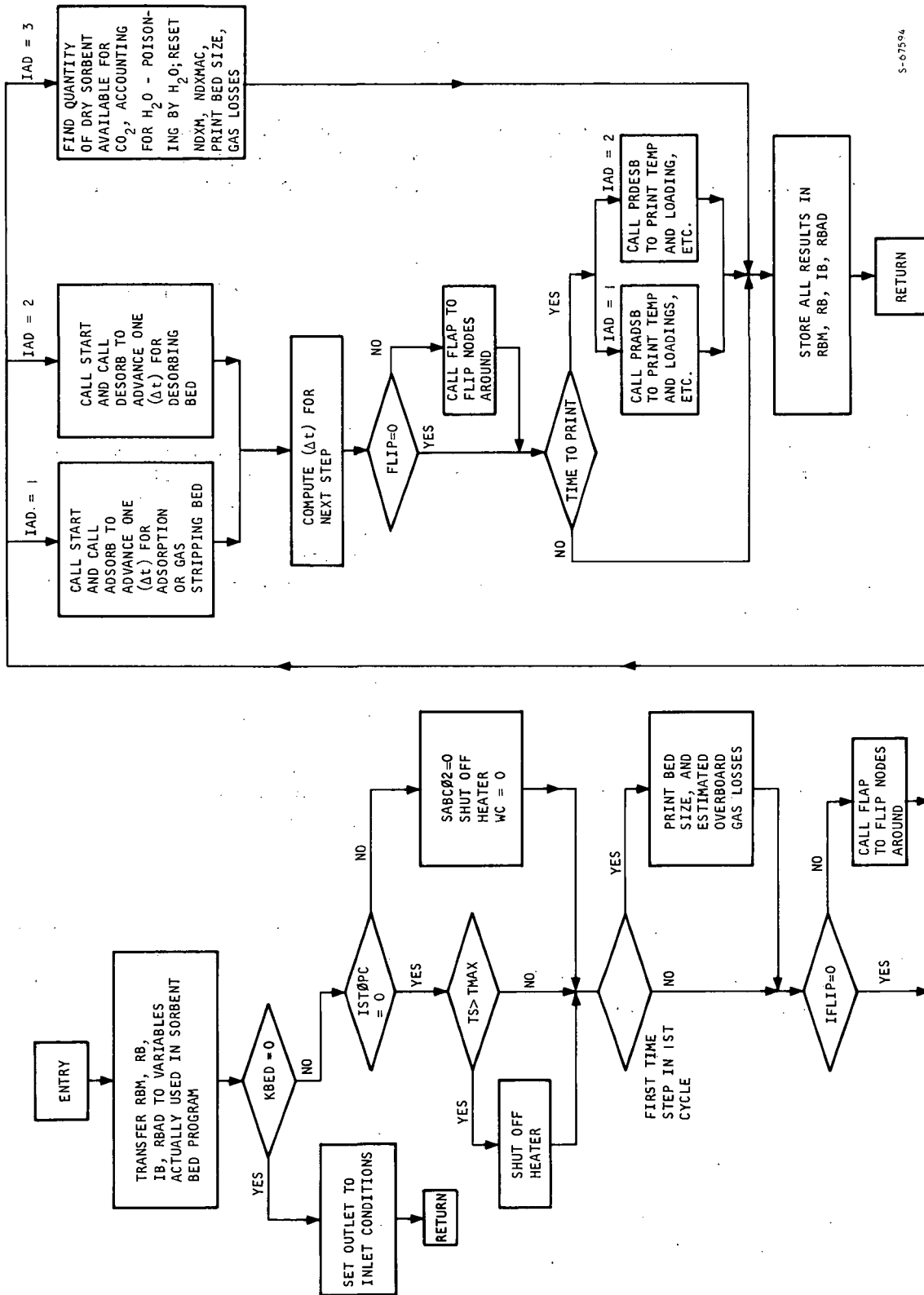
ID = Index identifying sorbate, 1 for CO₂, 2 for H₂O, 3 for N₂,
4 for O₂.

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.





S-67594

Figure A-1. Logic Diagram for Subroutine BED4

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

T = Temperature, °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, °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 $H_2O_T(I)$, $I = 1$ 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 ₂ O)	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, 62353 , 1

```

000001      SUBROUTINE ADSORB
000002      COMMON/AD/ TG(20),PH201,TGI,PA,PK(2,20),PC021,TS(20)
000003      1,TC(20),TX(20),TS1(20),TS2(20),TX1(20),TX2(20),TC1(20),
000004      2,TC2(20),W(4,20),PT(20),GMR,GMW,GVIS,PN2,P02,
000005      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000006      4,AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000007      5,CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000008      6,POUT(10),TIMET(10),WTACMS,WTSG,PUMP(10),VPUMP(10),CPP(20),
000009      7,NPSET(5),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000010      8      HXG(20),HXS(20),HXC(20),HSG(20),
000011      9,SK(20),TKX(20),DH(20),DJF(20),GK(20),UC(20),T268,TOTC02,TOTH20,
000012      1,SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000013      1TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VCO2A,SABC02,TC02A,
000014      1RS1(20,9),A(20),F(20),C(20),VS(20),DVS1(20),RS(20),
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000017      3,FR(2,20),P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000018      4(20,4),C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000019      5      WM(2),TIME,CYCLE,DT0,DTMAX,WI,TI,PC02C,
000020      6,VOLCAB,RCO2C,
000021      7,NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000023      1      CP1,CP2,X,C1P,C2P,C3P,D1P
000024      DIMENSION AS(20)
000025      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
000026      1,HGS)
000027      DATA RGAS/554./
000028
000029      C      NDR=NDR4-1
000030      DO 21 N=1,NDX1
000031      AS(N)=4.*3.1416*RS(N)**2
000032      I=N
000033      DO 20 NR=1,NDR4
000034      C1(NR,N)=-CR2(I,NR)
000035      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
000036      20 C3(NR,N)=-CR3(I,NR)
000037
000038      C
000039      C      B(1,N)=C3(1,N)/C2(1,N)
000040      DO 21 J=2,NDR
000041      21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
000042      NDX=NDX1-1
000043      C      TO TEMPORARILY STORE SURFACE LOADING
000044      DO 50 N=1,NDX1
000045      50 WS(N)=W(NDR4,N)
000046      IF (NTEMP.EQ.0) GO TO 111
000047
000048      C      TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
000049      DO 12 N=1,NDX1
000050      I=IFN(N,NDXM)
000051      CS2(N)=DT/CPS(N)/RHOSB(N)*ASG(N)*GK(N)*WM(I)*DH(N)
000052      CS1(N)=CS2(N)
000053      IF (N.EQ.1) GO TO 13
000054      IF (N.EQ.NDX1) GO TO 14
000055      S1=SK(N)/DX**2*(TS(N-1)-2.*TS(N)+TS(N+1))
000056      GO TO 15
000057      13 S1=SK(1)/DX**2*(TS(2)-TS(1))
000058      GO TO 15

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000059      14 S1=SK(NDX1)/DX**2*(TS(NDX)-TS(NDX1))
000060      15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+
000061      1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
000062      RATIO = (DT+DT0)/DT
000063      T=(DT+DT0)/CPS(N)/RHOSB(N)
000064      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000065      CS1(N)=RATIO*CS1(N)/(1.+T1)
000066      CS2(N)=RATIO*CS2(N)/(1.+T1)
000067      DS(N)=RATIO*DS(N)
000068      DS(N)= (DS(N)-T1*TS2(N))/(1.+T1)
000069      12 CONTINUE
000070      GO TO 110
000071      111 DO 112 N= 1, NDX1
000072      CS1(N)=0.
000073      CS2(N)=0.
000074      DS(N)=0.
000075      TS(N)=T268.
000076      TC(N)=T268
000077      TX(N)=T268
000078      TG(N)=T268
000079      112 CONTINUE
000080      110 CONTINUE
000081      C
000082      C TO CALCULATE PARTIAL PRESSURE OF ADSORBATE IN GAS STREAM
000083      C
000084      DO 24 N=1,NDX1
000085      I=IFN(N,NDXM)
000086      C TO CALCULATE P1,P2,P3
000087      WSURF=W(NDR4,N)
000088      CALL EQPWT(I,IDSORB(N),1,PSURF,WSURF,TS2(N))
000089      CALL EQPWT(I,IDSORB(N),1,PS1, WSURF,(TS2(N)+0.02))
000090      DPKDTS=(PS1-PSURF)/0.02
000091      CALL EQPWT(I,IDSORB(N),1,PS2,(WSURF+1.E-5),TS2(N))
000092      DPKDWK=(PS2-PSURF)/1.E-5
000093      G=1.+CS2(N)*DPKDTS
000094      P1(N)=(PSURF +DS(N)*DPKDTS)/G
000095      P2(N)=DPKDWK/G
000096      P3(N)=CS1(N)/G*DPKDTS
000097      C
000098      C2(NDR4,N)=CR1(N,NDR4)/DT+CR2(N,NDR4)+WM(I)*GK(N)*P2(N)*AS(N)
000099      C3(NDR4,N)=0.0
000100      DO 23 NR=1,NDR4
000101      23 D1(NR,N)=CR1(N,NR)/DT*W(NR,N)
000102      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(N)
000103      D2(N)=AS(N)*WM(I)*GK(N)*(1. -P3(N))
000104      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))
000105      Q(1,N)=D1(1,N)/C2(1,N)
000106      DO 24 J=2,NDR4
000107      24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
000108      C
000109      DO 25 N=1,NDX1
000110      I=IFN(N,NDXM)
000111      CP1(N)=ASG(N)*GK(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
000112      25 CP2(N)=ASG(N)*GK(N)*(P2(N)*D2(N)+P3(N)-1.0)
000113      PK(1,NDX1+1) = PCO2I
000114      PK(2,NDX1+1) = PH2OI
000115      DO 26 N=1,NDX1
000116      N1=NDX1+1-N
000117      I=IFN(N1,NDXM)
000118      PK(I,N1) = (PK(I,N1+1)/DX+CP1(N1)/A(N1))

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```

000119          1          /((1./DX-CP2(N1)/A(N1)))
000120          IF (I.EQ.1)J=2
000121          :IF(I.EQ.2)J=1
000122          PK(J,N1)=PK(J,N1+1)
000123          20 CONTINUE
000124          C
000125          C
000126          C
000127          C      TO CALCULATE SORBENT LOADING
000128          C
000129          DO 30 N=1,NDX1
000130          I=IFN(N,NDXM)
000131          W(NDR4,N)=Q(NDR4,N)+D2(N)*PK(I,N)
000132          DO 30 J=2,NDR4
000133          L=NDR4+1-J
000134          30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
000135          C
000136          C
000137          IF( NTEMP .EQ. 0) RETJRN
000138          C      TO CALCULATE SORBENT, GLYCOL, HX CORE AND GAS TEMPERATURES
000139          C
000140          CALL TSCRBA
000141          CALL TGLCOL(TC,NDX1,UC,RHOC,CPC,CX,AXC,HXC,T268,TX,DX,DT,
000142          1AVC,NOG ,DTO,TS1,TS2,TX1,TX2,TC1,TC2)
000143          CALL HXCORE
000144          CALL GASTA(GMR,CPG,ABED,NDX1,TGI,ASG,HSG,AXG,HXG,DX,TG,TS,TX)
000145          RETURN
000146          END

```



* ELT BED4,1,710720, 31270 , 1

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000001      SUBROUTINE BED4 (IBED, IFLIP, IAD, RBM, RB, IB, RBAD, ISTOPC, KBED)
000002      COMMON/AD/ TG(20), PH201, TGI, PA, PK(2,20), PC021, TS(20)
000003      1, TC(20), TX(20), TS1(20), TS2(20), TX1(20), TX2(20), TC1(20),
000004      2 TC2(20), W(4,20), PT(20), GMR, GMW, GV15, PN2, PO2,
000005      3 ABED(20), AVC(20), ASG(20), ASX(20), AGX(20), AXC(20),
000006      4 AVX(20), RHOG(20), RHOSB(20), RHOS(20), RHOC(20), RHOX(20),
000007      5 CPG(20), CPC(20), CPX(20), CPS(20), DX, CPL(2), DP(20),
000008      6 POUT(10), TIMET(10), WTACMS, WTSG, PUMP(10), VPUMP(10), CPP(20),
000009      7 NPSET(3), NDR4, NDXMAC, NBCOUT, NDX1, NDXM, NOG, IDSORB(20),
000010      8 HXG(20), HXS(20), HXC(20), HSG(20),
000011      9 SK(20), TKX(20), DH(20), DJF(20), GK(20), UC(20), T268, TOTCO2, TOTH20,
000012      1 SUMPTM, AVMSL1, AVSGL1, HTR(20), TMAX,
000013      1 TOTKWH, HTR1(20), WC, TOTWTC, WCC, PC02A, VCO2A, SABCO2, TCO2A,
000014      1 RS1(20,9), A(20), F(20), C(20), VS(20), DVS(20), DVS1(20), RS(20),
000015      1 UG(20), PS(20), DS(20), CS1(20), CS2(20), C1(4,20), C2(4,20), D1(4,20),
000016      2 D2(20), PC1(20), PC2(20), PC3(20), C1P(20), C2P(20), C3P(20), D1P(20),
000017      3 FR(2,20), P1(20), P2(20), P3(20), WS(20), CR1(20,4), CR2(20,4), CR3
000018      4(20,4), C3(4,20), B(4,20), G(4,20), CP1(20), CP2(20), X(20), VOIDF(20),
000019      5 WM(2), TIME, CYCLE, DTO, DTMAX, WI, TI, PC02C,
000020      6 VOLCAB, RC02C,
000021      7 NCYCLT, NPRINT, NCYCLE, VDTCON, NTEMP, NSTART, NPR, DT, DTT(4), SABCOS
000022      DOUBLE PRECISION C1, C2, D1, D2, PC1, PC2, PC3, P1, P2, P3, C3, G, B,
000023      1 CP1, CP2, X, C1P, C2P, C3P, D1P
000024      DIMENSION RBM(1), RB(1), IB(1), RBAD(1), KBED(1)
000025      DIMENSION WN(20)
000026      C IFLIP = 0, NO FLIP, IFLIP=1, FLIP WILL BE CALLED
000027      DATA ISTART/0/
000028      C
000029      DO 110 N=1,349
000030      110 TG(N)=RBM(N)
000031      DO111 N=1, 405
000032      111 ABED(N)=RB(N)
000033      DO112 N= 1,29
000034      112 NPSET(N)=IB(N)
000035      DO 13 N=1,251
000036      13 HXG(N)=RBAD(N)
000037      IF (KBED (IBED) ,EQ. 0) GO TO 90
000038      8976 FORMAT (I25)
000039      NDX10=NDX1
000040      NDX1=NDX10
000041      SABCO2=SARCOS
000042      IF (ISTOPC .NE. 0) SABCO2=0.0
000043      DO 1311 N= 1, NDX1
000044      HTR(N)=HTR1(N)
000045      IF (ISTOPC .NE. 0) GO TO 3198
000046      IF (TS(N) .GT. TMAX) GO TO 3198
000047      GO TO 1311
000048      3198 DO 411 J= 1, NDX1
000049      411 HTR(J) = 0.0
000050      GO TO 66
000051      1311 CONTINUE
000052      66 CONTINUE
000053      ISTART=ISTART+1
000054      IF (TIME .LT. 1.1E-5) GO TO 80
000055      GO TO 81
000056      80 SUMPTM=0.0
000057      TOTKWH=0.0
000058      TOTCO2=0.0

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* THESE TWO CARDS ARE ENTROPY GENERATORS



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000059      TOTHTC=0.
000060      TOTHTC=U.0
000061      IF(ISTART .GT. 4) GO TO 81
000062
C
000063      ASSIGN 82 TO NPR5BR
000064      GO TO 183
000065
C
000066      82 CONTINUE
000067
000068      81 WC=WCC
000069      IF(ISTOPC.NE.0) WC=0.
000070      DO 801 N=1,NDX1
000071      AC=ABEQ(N)*ASX(N)/AVC(N)
000072      801 UC(N)=WC/AC/RHOC(N)
000073      IF(IFLIP.NE.0) CALL FLAP
000074      15 GO TO (16,17,18), IAD
000075      16 CALL START
000076      CALL ADSORB
000077      SUMPTH= SUMPTH+PK(2,1)*DT
000078      GO TO 19
000079      17 CALL START
000080      CALL DESORB
000081      19 ADT = DTMAX
000082      DO 60 N=1,NDX1,4
000083      ADT2=W1 /((ABS(W(NDR4,N))-WS(N))+1.E-9)*DT
000084      IF(ADT2.LT. ADT) ADT=ADT2
000085      ADT2=T1/((ABS(TS(N)-TS2(N))+1.E-9)*DT*2.0
000086      IF(ADT2.LT. ADT) ADT=ADT2
000087      ADT2=T1/((ABS(TX(N)-TX2(N))+1.E-9)*DT*2.0
000088      IF(ADT2.LT. ADT) ADT=ADT2
000089      ADT2=T1/((ABS(TC(N)-TC2(N))+1.E-9)*DT*2.0
000090      IF(ADT2.LT. ADT) ADT=ADT2
000091      60 CONTINUE
000092      IF(ADT.LT. 1.E-5)ADT=1.E-5
000093      DTT(IBED)=ADT
000094      DO 21 N=1,NDX1
000095      TS2(N)=TS1(N)
000096      TX2(N)=TX1(N)
000097      TC2(N)=TC1(N)
000098      21 CONTINUE
000099      IF(IFLIP.NE.0) CALL FLAP
000100      DO 211 N= 1, NDX1
000101      211 TOTKWH=TOTKWH+DT*HTR(N)/3410.
000102      TOTHTC=TOTHTC+WC*CPC(VOG)*DT*(T268-TC(NDX1))
000103      IF(
000104      1 ((TIME.LT.1.1E-5).OR.(TIME.GE.CYCLE).OR. (NPR/NPRINT*NPRINT
000105      2.EQ.NPR)).AND. (NCYCLE.GE. NSTART)) GO TO 130
000106      GO TO 33
000107
C
000108      130 CONTINUE
000109      GO TO(31,32), IAD
000110
C
000111      31 CALL PRADS(BED)
000112      GO TO 33
000113      32 CALL PRDES(BED)
000114      GO TO 33
000115      33 DO 20 N=1,349
000116      20 RBM(N)=TG(N)
000117      DO 23 N=1,251
000118      23 RBAD(N)=HXG(N)

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000119      DO 41 N= 1, 405
000120      41 RB(N)=ABED(N)
000121      DO 181 N=1,29
000122      181 IH(N)=NPSET(N)
000123      RETURN
000124      18 SUMCOS=0.
000125      IF(NDXM.EQ.NDX1)CALL EXIT
000126      NDB=NDXM+1
000127      DO 42 N=NDB,NDX1
000128      CALL EQPWT(1,IDSORB(N),2,3.,WN1,70.)
000129      WN(N)=WN1*ABE(N)*DX*RHOSB(N)
000130      SUMCOS=SUMCOS+WN(N)*FCOAD(IDSORB(N),W(1,N))
000131      42 CONTINUE
000132      DO 43 N=NDB,NDX1
000133      DIF(N)=DIF(1)
000134      GK(N)=GK(1)
000135      DH(N)=DH(1)
000136      IF(SUMCCS-WN(N))46,44,44
000137      46 CONTINUE
000138      FRHO=SUMCOS/WN(N)
000139      DRHO=RHOSB(N)*(1.-FRHO)
000140      RHOSB(N)= RHOSB(N)*FRHO
000141      IF(N.LT.NDX1) GO TO 51
000142      RHOSB(N+1)=DRHO
000143      GO TO 50
000144      51 NTDB=NDX1-N
000145      DRHO1=DRHO/NTDB
000146      K1=N+1
000147      DO 53 K=K1,NDX1
000148      53 RHOSB(K)=RHOSB(K)+DRHO1
000149      50 NDXM=N
000150      NDXMAC=N
000151      ASG(N)=ASG(1)*RHOSB(N)/RHOSB(1)
000152      IF(N.EQ.NDX1)NDX1=NDX1+1
000153      GO TO 47
000154      44 SUMCOS=SUMCOS+WN(N)
000155      ASG(N)=ASG(1)*RHOSB(N)/RHOSB(1)
000156      IF(SUMCOS.LT.1.E-10) GO TO 50
000157      43 CONTINUE
000158      47 CONTINUE
000159      49 CONTINUE
000160      ASSIGN 83 TO NPRSBR
000161      GO TO 183
000162      83 CONTINUE
000163      GO TO 33
000164      90 CONTINUE
000165      PK(1,1)=PC02I
000166      91 PK(2,1)=PH20I
000167      TG(1)=TGI
000168      GO TO 33
000169      C
000170      C
000171      C PRSBWT ROUTINE CCCCCCCCC
000172      183 CONTINUE
000173      WCC=WC
000174      N1=NDXM+1
000175      VMS = 0.0
000176      WTMS=0.0
000177      VSG=0.0
000178      WTSG=0.0

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000179      IF(NDXH .EQ. 0) GO TO 11
000180      DO 10 N= 1, NDXM
000181      VMS=VMS+DX*ABED(N)
000182      WTMS=WTMS+DX*ABED(N)*RHOSR(N)
000183 10 CONTINUE
000184 11 CONTINUE
000185      IF((NDX1-NDXM) .EQ. 0) GO TO 31
000186      DO 30 N= N1,NDX1
000187      VSG=VSG+DX*ABED(N)
000188      WTSG=WTSG+DX*ABED(N)*RHOSB(N)
000189 30 CONTINUE
000190 31 CONTINUE
000191      WTACMS=0.0
000192      WN2L=0.0
000193      W02L=0.0
000194      TN2=70.
000195      T02=70.
000196      IF(NDXMAC .EQ. 0) GO TO 12
000197      DO 70 N= 1, NDXMAC
000198      CALL EQPWT(3,IDSORB(N),2,PN2,WN2,TN2)
000199      CALL EQPWT(4,IDSORB(N),2,P02,W02,T02)
000200      WN2L=WN2L+DX*ABED(N)*RHOSB(N)*WN2
000201      W02L=W02L+DX*ABED(N)*RHOSB(N)*W02
000202 70 WTACMS=WTACMS + DX*ABED(N)*RHOSR(N)
000203 12 CONTINUE
000204      WRITE(6,503) IBED
000205 503 FORMAT(1H1////7H BED NO I2//// 20H VOLUME AND WEIGHT // )
000206      WRITE(6,500) VMS,WTMS,WTACMS,VSG,WTSG
000207 500 FORMAT(
000208 1' BULK VOLUME OF CO2 SORBENT (CU FT) 'F8.4/
000209 2' WEIGHT OF CO2 SORBENT (LB) 'F8.4/
000210 3' WEIGHT OF ACTIVE CO2 SORBENT (LB) 'F8.4//
000211 4' BULK VOLUME OF DESICCANT (CU FT) 'F8.4/
000212 5' WEIGHT OF DESICCANT (LB) 'F8.4)
000213 C
000214      CALL START
000215      WN2V=0.
000216      W02V=0.0
000217      DO 600 N=1,NDX1
000218      VOLN=ABED(N)*DX*VOIDF(N)
000219      WN2V=WN2V+28./359.*492./(70.+460.)/760.*PN2*VOLN
000220      W02V=W02V+32./359.*492./(70.+460.)/760.*P02*VOLN
000221 600 CONTINUE
000222      WN2L=WN2L+WN2V
000223      W02L=W02L+W02V
000224      RN2L=WN2L/CYCLE/2.0
000225      R02L=W02L/CYCLE/2.
000226      WRITE(6,505) RN2L,R02L
000227 505 FORMAT(///// ESTIMATED CABIN GAS LOSSES'//
000228 1' NITROGEN LOSS (LB/HR) 'F8.4/
000229 2' OXYGEN LOSS (LB/HR) 'F8.4)
000230      GO TO NPRSBR
000231      END

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-----END CUR



• FLT DESORB.1,710719, 62340 , 1

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000001      SUBROUTINE DESORB
000002      C
000003      COMMON/AD/ TG(20),PH201 ,TGI ,PA ,          PK (2,20),PC021 ,TS (20)
000004      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000005      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,
000006      3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000007      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000008      5PCP(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000009      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000010      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000011      8          HXG(20),HXS(20),HXC(20),HSG(20),
000012      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTC02,TOTH20,
000013      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000014      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABC02, TC02A,
000015      1RS1(20,9),          A(20),F(20),C(20),VS(20),OVS(20),OVS1(20),RS(20),
000016      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000017      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000018      3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000019      4(20,4),          C3(4,20),B(4,20),G(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000020      5          WM(2),TIME,CYCLE,DT0,          DTMAX,WI,TI,PC02C,
000021      6VOLCAB,RC02C,
000022      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SARCOS
000023      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,G,B,
000024      1          CP1,CP2,X,          C1P,C2P,C3P,D1P
000025      DIMENSION AS(20), PD(20)
000026      DIMENSION P4(20),VIST(2)
000027      DOUBLE PRECISION G,DPKDT5,DPKDWK,PD
000028      EQUIVALENCE (ASX,AXS),(AGX,AXG),(ASG,AGS),(HXS,HSX),(HXG,HGX),(HSG
000029      1,HGS)
000030      EQUIVALENCE (PS,P4)
000031      DIMENSION SPT(10), PET(10)
000032      EQUIVALENCE (SPT,VPUMP),(PET,PUMP)
000033      DATA VIST/0.014, 0.009/
000034      DATA RGAS/554./
000035      C
000036      IF(TIME .LE.1.E-5)PF13=3.
000037      NDR=NDR4-1
000038      DO 21 N=1,NDX1
000039      J=2
000040      P4(N)=PT(N)
000041      AS(N)=4.*3.1416*RB(N)**2
000042      I=IFN(N,NDXM)
000043      IF( I .EQ. 2) J=1
000044      VIS= X(N)*VIST(I)*(1.-X(N))*VIST(J)
000045      F(N)=2.494E-4*PT(N)**0.795*(VIS/0.0174)
000046      DO 20 NR=1,NDR4
000047      I=N
000048      C1(NR,N)=-CR2(I,NR)
000049      C2(NR,N)=CR1(I,NR)/DT+CR2(I,NR)+CR3(I,NR)
000050      20 C3(NR,N)=-CR3(I,NR)
000051      C
000052      C
000053      B(1,N)=C3(1,N)/C2(1,N)
000054      DO 21 J=2,NDR
000055      21 B(J,N)=C3(J,N)/(C2(J,N)-C1(J,N)*B(J-1,N))
000056      NDX=NDX1-1
000057      C TO TEMPORARILY STORE SURFACE LOADING
000058      DO 50 N=1,NDX1

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000059      >D WS(N)=W(NDR4,N)
000060      C
000061      C   TO CALCULATE CS1,CS2,DS FOR SORBENT HEAT BALANCE EQUATION
000062      IF (NTEMP.EQ. 0 ) GO TO 111
000063      DO 12 N=1,NDX1
000064      I=IFN(N,NDXM)
000065      CS2(N)=DT/CPS(N)/RHOSB(N)*ASG(N)*GK(N)*WM(I)*DH(N)
000066      CS1(N) = CS2(N)*X(N)
000067      IF (N.EQ.1) GO TO 13
000068      IF (N.EG.NDX1) GO TO 14
000069      S1=SK(N)/DX**2*(TS(N-1)-2.*TS(N)+TS(N+1))
000070      GO TO 15
000071      13 S1=SK(1)/DX**2*(TS(2)-TS(1))
000072      GO TO 15
000073      14 S1=SK(NDX1)/DX**2*(TS(NDX)-TS(NDX1))
000074      15 DS(N)=DT/CPS(N)/RHOSB(N)*(S1+ASG(N)*HSG(N)*(TG(N)-0.5*TS2(N))+
000075      1ASX(N)*HXS(N)*(TX(N)-0.5*TS2(N)))
000076      RATIO = (DT+DT0)/DT
000077      T=(DT+DT0)/CPS(N)/RHOSB(N)
000078      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000079      CS1(N)=RATIO*CS1(N)/(1.+T1)
000080      CS2(N)=RATIO*CS2(N)/(1.+T1)
000081      DS(N)=RATIO*DS(N)
000082      DS(N)= (DS(N)-T1*TS2(N))/(1.+T1)
000083      12 CONTINUE
000084      GO TO 110
000085      111 DO 112 N=1,NDX1
000086      CS1(N)=0.
000087      CS2(N)=0.
000088      DS(N)=0.
000089      TS(N)=T268
000090      TC(N)=T268
000091      TX(N)=T268
000092      TG(N)=T268
000093      112 CONTINUE
000094      110 CONTINUE
000095      C
000096      C   TO CALCULATE TOTAL PRESSURE
000097      C
000098      DO 24 N=1,NDX1
000099      I=IFN(N,NDXM)
000100      C   TO CALCULATE P1,P2,P3
000101      WSURF=W(NDR4,N)
000102      CALL EQPWT(I,IDSORB(N),1,PSURF,WSURF,TS2(N))
000103      CALL EQPWT(I,IDSORB(N),1,PS1, WSURF,(TS2(N)+0.02))
000104      DPKDTS=(PS1-PSURF)/0.02
000105      CALL EQPWT(I,IDSORB(N),1,PS2,(WSURF+1.E-5),TS2(N))
000106      DPKDWK=(PS2-PSURF)/1.E-5
000107      G=1.+CS2(N)*DPKDTS
000108      P1(N)=(PSURF +DS(N)*DPKDTS)/G
000109      P2(N)=DPKDWK/G
000110      P3(N)=CS1(N)/G*DPKDTS
000111      C
000112      C2(NDR4,N)=CR1(N,NDR4)/DT+CR2(N,NDR4)+WM(I)*GK(N)*P2(N)*AS(N)
000113      C3(NDR4,N)=0.0
000114      DO 23 NR=1,NDR4
000115      23 D1(NR,N)=CR1(N,NR)/DT*W(NR,N)
000116      D1(NDR4,N)=D1(NDR4,N)-WM(I)*GK(N)*(P1(N)-P2(N)*W(NDR4,N))*AS(N)
000117      D2(N)=AS(N)*WM(I)*GK(N)*(X(N) -P3(N))
000118      D2(N)=D2(N)/(C2(NDR4,N)-C1(NDR4,N)*B(NDR4-1,N))

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000119      Q(1,N)=D1(1,N)/C2(1,N)
000120      DO 24 J=2,NDR4
000121      24 Q(J,N)=(D1(J,N)-C1(J,N)*Q(J-1,N))/(C2(J,N)-C1(J,N)*B(J-1,N))
000122      C
000123      C   COEFFICIENTS FOR P-EQUATION
000124      DO 25 N=2,NDX
000125      25 PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1
000126      1)/F(N+1) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(2.*DX)
000127      N=1
000128      PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N+1)*C(N+1)*ABED(N+1
000129      1)/F(N+1) - VOIDF(N )*C(N )*ABED(N )/F(N ))/(1.*DX)
000130      N= NDX1
000131      PC2(N) = PT(N)/(VOIDF(N)*C(N)*ABED(N))*(VOIDF(N )*C(N )*ABED(N
000132      1)/F(N ) - VOIDF(N-1)*C(N-1)*ABED(N-1)/F(N-1))/(1.*DX)
000133      DO 26 N=1,NDX1
000134      PC1(N)=PT(N)/F(N)
000135      26 PC3(N)=PT(N)/C(N)/VOIDF(N)*ASG(N)*GK(N)
000136      C
000137      DO 27 N=1,NDX1
000138      CP1(N)=PC3(N)*(P1(N)+P2(N)*(Q(NDR4,N)-W(NDR4,N)))
000139      CP2(N)=PC3(N)*(P2(N)+P3(N) -X(N))
000140      C1P(N)=-PC1(N)/DX/DX+PC2(N)/2./DX
000141      C2P(N)=1./DT+2.*PC1(N)/DX/DX-CP2(N)
000142      C3P(N)=-PC1(N)/DX/DX-PC2(N)/2./DX
000143      27 D1P(N)=PT(N)/DT+CP1(N)
000144      C
000145      C   BOUNDARY CONDITION FOR P-EQUATION
000146      C
000147      C2P(1)=C2P(1)*C1P(1)
000148      C1P(1)=0.
000149      GO TO (55,56,58,58), NBCOUT
000150      58 CONTINUE * PUMP CHARACTERISTIC GIVEN
000151      POPI=PCO2A*51.7/PT(NDX1)
000152      CALL LAGIN2( 58,PUMP,10,2,POPI,VPUMP1,VPUMP)
000153      VPUMP1=VPUMP1*(TG(NDX1)+460.)/(TCO2A+460.)
000154      IF(VPUMP1 .LT. 0.0) VPUMP1=0.00
000155      CEXIT=VPUMP1*60./(ABED(NDX1)*VOIDF(NDX1))/PT(NDX1)
000156      GO TO 59
000157      C
000158      55 CONTINUE
000159      EMW=X(NDX1)*WM(2)+(1.-X(NDX1))*WM(1)
000160      EVIS=X(NDX1)*VIST(2)+(1.-X(NDX1))*VIST(1)
000161      EVIS=EVIS*0.01
000162      SQTM= SQRT( (TG(NDX1)+460.)/1.8/EMW)
000163      DIA=6.0
000164      TOTL=127.
000165      PTAVG=0.5*(PT(NDX1)+PF13)
000166      EV=3.269E-2*PTAVG* DIA**4/TOTL/EVIS+
000167      13.81*DIA**3/TOTL*(SQTM+0.147*PTAVG* DIA/EVIS)
000168      2/(SQTM+0.181*PTAVG* DIA/EVIS)
000169      EV=EV*3600./28.316
000170      EV1=EV
000171      N1=1
000172      91 CONTINUE
000173      QF=(PT(NDX1)-PF13)*EV
000174      CALL LAGIN2(58,PET,10,2,PF13,SP,SPT)
000175      DGF=QF-SP*PF13
000176      CALL NEWTO2(N1,NGO,PF13,DGF,PF130,DGFO,1.E-3,PT(NDX1),0.0111)
000177      GO TO (91,92), NGO
000178      92 CONTINUE

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000179      EV=SP*EV/(SP+EV)
000180      C2P(NDX1)=C2P(NDX1)+C3P(NDX1)*(1.-EV*F(NDX1)*DX/V0IDF(NDX1)/ABED
000181      1(NDX1)/PT(NDX1))
000182      C3P(NDX1)=0.000
000183      GO TO 57
000184
C
000185      59 C2P(NDX1) = C2P(NDX1)+C3P(NDX1)*(1.-DX*F(NDX1)*CEXIT)
000186      C3P(NDX1)=0.0
000187      GO TO 57
000188      56 CONTINUE
000189      C PRESSURES ARE SET
000190
C
000191      DO 561 K= 1, 3
000192      IF(NPSET(K) .EQ. 0) GO TO 561
000193      NP=NPSET(K)
000194      C1P(NP)=0.0
000195      C2P(NP)=1.0
000196      C3P(NP)=0.0
000197      CALL LAGIN2(10,TIME,10,2,TIME,D1PNP ,POUT)
000198      D1P(NP)=D1PNP
000199      561 CONTINUE
000200      57 CONTINUE
000201      CALL FDEQID(C1P,C2P,C3P,D1P,PD,NDX1)
000202      DO 34 N=1,NDX1
000203      IF(PD(N) .LE. 0.) PD(N) = 1.E-3
000204      34 PT(N)=PD(N)
000205
C
000206      TO CALCULATE SORBENT LOADING
000207
C
000208      DO 30 N=1,NDX1
000209      W(NDR4,N)=Q(NDR4,N)+D2(N)*PT(N)
000210      DO 30 J=2,NDR4
000211      L=NDR4+1-J
000212      30 W(L,N)=Q(L,N)-B(L,N)*W(L+1,N)
000213
C
000214      TO CALCULATE STREAM COMPOSITION
000215
C
000216      FR(1,1) = 0.0
000217      FR(2,1)=0.
000218      FR2=0.0
000219      DO 31 N=1,NDX1
000220      I=IFN(N,NDXM)
000221      TEMP =C(N)*V0IDF(N)
000222      1/P4(N)*ABED(N) *DX*(CP1(N)+CP2(N)*PT(N))
000223      IF(1.EQ.1)J=2
000224      IF(1.EQ.2)J=1
000225      IF(N .EQ. 1) GO TO 200
000226      FR(J,N)=FR(J,N-1)
000227      FR(1,N)=TEMP+FR(1,N-1)
000228      IF( NDXM .EQ. 0) GO TO 202
000229      IF (1 .EQ. 1) GO TO 202
000230      IF(NPSET(2) .NE. 0) GO TO 202
000231      GO TO 201
000232      200 FR(1,1) = TEMP
000233      202 X(N) = 1.0
000234      GO TO 31
000235      201 CONTINUE
000236      CT=ABED(N)*DX*ASG(N)*GK(N)
000237      FRT= FR(1,N)+FR(2,N)+1.E-10
000238      PSURF = P1(N)+P2(N)*(W(NDR4,N)-WS(N))+P3(N)*PT(N)

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000239      X(N)=((FR(2,N-1)+CT*PSURF      )/FRT/
000240      1 (1.+CT*PT(N)/FRT)
000241      IF(X(N) .LT. 0.0) X(N)=0.0
000242      IF(X(N) .GT. 1.0) X(N)=1.0
000243      31 CONTINUE
000244      DO 33 N=1,NDX1
000245      C(N) = (PT(N)/RGAS/(TG(N)+460)+C(N))/2.0
000246      I = IFN (N,NDXM)
000247      IF (I.EQ.1) J=2
000248      IF (I.EQ.2) J=1
000249      RHOG(N)=C(N)*(X(N)*WM(I)+(1.-X(N))*WM(J))
000250      UG(N)=(FR
000251      1 (1,N)*WM(1)+FR(2,N)*WM(2))/RHOG(N)/ABED(N)/VOIDF(N)
000252      33 CONTINUE
000253      IF( NTEMP .EQ. 0) RETURN
000254      C
000255      C
000256      C      TO CALCULATE SORBENT TEMPERATURES
000257      CALL TSCRB
000258      D9=DT
000259      CALL TGLCOL(TC,NDX1,UC,RHOG,CPC,CX,AXC,HXC,T268,TX,DX,D9,
000260      1AVC, NOG ,DT0,TS1,TS2, TX1, TX2, TC1, TC2)
000261      CALL HXCORE
000262      CALL GAST(DX,RHOG,CPC,UG,TS,TX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF)
000263      100  FORMAT(8G12.3)
000264      DESRAT=FR(1,NDX1)
000265      IF(NBCOUT .EQ. 3) GO TO 101
000266      IF(NBCOUT .EQ. 4) GO TO 1018
000267      RETURN
000268      101 CONTINUE
000269      DPCO2A=(DESRAT-SABCO2/44.)*DT*RGAS*(TCO2A+460.)/VCO2A/51.7
000270      PCO2A=PCO2A+DPCO2A
000271      RETURN
000272      1018 CONTINUE
000273      DVCO2A = (DESRAT -SABCO2/44.0)*DT*RGAS*(TCO2A+460.0)/PCO2A/51.7
000274      VCO2A=VCO2A+DVCO2A
000275      RETURN
000276      END

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ELT EQPWT,1,710712, 56799 , 1

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000001      SUBROUTINE EQPWT(ID,IDSORB,KPW,P,W,T)
000002      C      KPW=1 = W,T TO FIND P
000003      C      KPW=2 = P,T TO FIND W
000004      C      PKEQ=EQUILIBRIUM PRESSURE IN MM HG
000005      C      W=LOADING IN LB ADSORBATE PER LB ADSORBENT
000006      C      T=TEMP IN DEG F
000007      C
000008      DIMENSION TTAB(10,25), WTAB(15,10,25), PTAB(15,10,25), NT(25)
000009      DIMENSION IDSMTX(5,5)
000010      C      NT(1) DATA FOR CO2 ON MOL SIEVE 5A
000011      C      NT(2) DATA FOR H2O ON MOL SIEVE 5A
000012      C      NT(3) DATA FOR H2O ON SILICA GEL
000013      C      NT(4) DATA FOR CO2 ON MOL SIEVE 13X
000014      C      NT(5) DATA FOR H2O ON MOL SIEVE 13X
000015      DATA IDSMTX/1.0,4.0,0.2,3.5, 0.0, 6.0,8.0,0.7,0.9,0.0,0.0,0.0,0.0/
000016      DATA JACK/0/
000017      DATA NT/25*0./
000018      C
000019      DATA NT(1)/6/
000020      DATA (TTAB(J,1),J=1,6)/392.,212.,122.,77.,51.,32./
000021      DATA (WTAB(I,1,1),I=1,15)/.001,.0018,.0021,.0025,.003,.0037,.004.,
000022      1.0045,.005,.0055,.0063,.007,.008,.0088,.0092/
000023      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.,
000024      15.,20.,30.,40.,50./
000025      DATA (WTAB(I,2,1),I=1,15)/.002,.0028,.004,.0047,.0052,.006,.007.,
000026      1.009,.01,.012,.013,.019,.025,.03,.034/
000027      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.,
000028      15.,20.,30.,40.,50./
000029      DATA (WTAB(I,3,1), I=1,15)/ 0.0009,0.0018,0.0025,0.0027,0.0043,
000030      10.0065,0.01,0.0145,0.0178,0.0265,0.0325,0.04,0.0485,0.057,0.07/
000031      DATA (WTAB(I,5,1),I=1,15)/0.002,0.005,0.008,0.0122,0.018,0.0255,
000032      10.0324,0.04,0.05,0.07,0.08,0.09,0.1,0.11,0.1177/
000033      DATA (WTAB(I,6,1),I=1,15)/0.0016,0.0035,0.0073,0.01,0.015,0.02,
000034      10.0277,0.04,0.05,0.06,0.077,0.09,0.1,0.11,0.12/
000035      DATA (PTAB(I,3,1),I=1,15)/.05,.1,.2,.3,.7,1.1,1.9,3.,4.,7.,
000036      110.,14.5,20.,26.,40./
000037      DATA (WTAB(I,4,1),I=1,15)/.0009,.0025,.0033,.006,.0093,.013,
000038      10.0174,.027,.0347,.041,.05,.06,.08,.0955,.103/
000039      DATA (PTAB(I,4,1),I=1,15)/.03,.06,.1,.2,.4,.7,1.,2.,
000040      13.,4.,5.6,7.7,13.,20.,26.5/
000041      DATA (PTAB(I,5,1),I=1,15)/0.02,.05,.1,.2,.4,.7,1.,1.5,
000042      12.17,3.9,5.,7.,10.,15.,20./
000043      DATA (PTAB(I,6,1),I=1,15)/0.01,.03,.06,.1,.2,.3,.5,.88,
000044      11.32,1.8,3.,4.65,6.6,9.5,15./
000045      C
000046      DATA NT(2)/6/
000047      DATA (TTAB(J,2),J=1,6)/392.,212.,167.,122.,77.,32./
000048      DATA (WTAB(I,1,2),I=1,15)/.004,.007,.01,.012,.015,.018,.02,.023,
000049      1.028,.038,.05,.071,.076,.081,.09/
000050      DATA (PTAB(I,1,2),I=1,15)/.01,.02,.05,.1,.2,.5,1.,2.,5.,10.,20.,
000051      150.,60.,75.,100./
000052      DATA (WTAB(I,2,2),I=1,15)/.02,.024,.026,.030,.036,.045,.051,.058,
000053      1.074,.091,.11,.135,.15,.16,.175/
000054      DATA (PTAB(I,2,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1.0,2.0,
000055      14.0, 10., 20., 40., 100./
000056      DATA (WTAB(I,3,2),I=1,15)/.027,.035,.038,.045,.057,.071,.08,.092,
000057      1.11,.125,.139,.149,.16,.18,.19/
000058      DATA (PTAB(I,3,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1.,2.,3.,4.,

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000059 110.,60.,120./
000060 DATA (WTAB(I,4,2),I=1,15)/.045,.058,.065,.078,.097,.115,.125,.135,
000061 1.145,.160,.165,.175,.180,.185,.188/
000062 DATA (PTAB(I,4,2),I=1,15)/.01,.02,.03,.05,.1,.2,.3,.5,1,.2,.3,.10,
000063 1,20.,60.,120./
000064 DATA (WTAB(I,5,2),I=1,15)/.083,.103,.115,.12,.14,.155,.159,.163,
000065 1.175,.18,.181,.182,.183,.184,.185/
000066 DATA (PTAB(I,5,2),I=1,15)/.01,.02,.03,.04,.1,.2,.3,.5,1,.2,.4,.7.,
000067 115.,40.,100./
000068 DATA (WTAB(I,6,2),I=1,15)/.135,.15,.155,.16,.167,.169,.173,.178,.18
000069 10.,.181,.183,.184,.185,.186,.187/
000070 DATA (PTAB(I,6,2),I=1,15)/.01,.02,.03,.04,.07,.10,.20,.50,1.5,3.0,
000071 17.0,15.0,30.0,70.0,100.0/
000072
000073 DATA NT(3)/5/
000074 DATA (TTAB(J,3),J=1,5)/160.,100.,60.,40.,10./
000075 DATA (WTAB(I,1,3),I=1,15)/.0018,.0026,.0031,.0057,.008,.01,.03,
000076 1.06,.10,.14,.20,.32,.45,.49,.50/
000077 DATA (PTAB(I,1,3),I=1,15)/.01,.05,.1,.4,1.0,1.95,9.42,23.6,44.8,
000078 167.2,101.8,200.,400.,700.,1000./
000079 DATA (WTAB(I,2,3),I=1,15)/.00305,.005,.0069,.009,.02,.05,.07,.11,
000080 1.17,.215,.32,.42,.50,.58,.59/
000081 DATA (PTAB(I,2,3),I=1,15)/.01,.05,.10,.2,.87,3.20,5.04,9.06,15.6,
000082 120.,30.,50.,100.,300.,700./
000083 DATA (WTAB(I,3,3),I=1,15)/.005,.008,.01,.02,.04,.05,.06,.10,.19,
000084 1.27,.405,.50,.55,.60,.64/
000085 DATA (PTAB(I,3,3),I=1,15)/.01,.03,.07,.206,.574,.79,1.02,2.04,4.7,
000086 17.23,15.,30.,50.,100.,300./
000087 DATA (WTAB(I,4,3),I=1,15)/.008,.0092,.01,.02,.03,.05,.07,.11,.27,
000088 1.40,.42,.48,.57,.67,.75/
000089 DATA (PTAB(I,4,3),I=1,15)/.01,.02,.03,.092,.17,.36,0.58,1.08,3.45,
000090 16.0,8.0,10.0,20.0,70.0,200.0/
000091 DATA (WTAB(I,5,3),I=1,15)/.014,.018,.022,.05,.08,.205,.28,.35,.42,
000092 1.50,.60,.70,.77,.80,.82/
000093 DATA (PTAB(I,5,3),I=1,15)/.01,.02,.03,.10,.20,.70,1.0,1.5,2.0,3.0,
000094 15.0,10.0,20.0,40.0,100.0/
000095
000096 DATA NT(4)/3/
000097 DATA (TTAB(J,4),J=1,3)/122.,77.,32./
000098 DATA (WTAB(I,1,4),I=1,15)/.00355,.0036,.00365,.0037,.0038,.0040,
000099 1.0045,.005,.0059,.0077,.011,.016,.020,.026,.037/
000100 DATA (PTAB(I,1,4),I=1,15)/.02,.03,.04,.05,.07,.10,.20,.30,.50,1.0,
000101 12.0,4.0,6.0,10.0,20.0/
000102 DATA (WTAB(I,2,4),I=1,15)/.0098,.01,.0105,.0115,.0124,.0133,.0150,
000103 1.0165,.018,.021,.033,.0415,.0475,.055,.064/
000104 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
000105 1.4,0.7,0.10,0.15,0.25,0/
000106 DATA (WTAB(I,3,4),I=1,15)/.018,.0187,.0191,.02,.0222,.0248,.0282,
000107 1.031,.033,.0355,.04,.05,.068,.078,.095/
000108 DATA (PTAB(I,3,4),I=1,15)/.002,.01,.02,.04,.10,.20,.40,.60,.80,1.,
000109 11.5,3.0,6.0,10.0,20.0/
000110
000111 DATA NT(5)/6/
000112 DATA (TTAB(J,5),J=1,6)/400.,300.,200.,122.,77.,35./
000113 DATA (WTAB(I,1,5),I=1,15)/.0001,.0002,.0005,.001,.002,.003,
000114 1.005,.01,.016,.022,.03,.041,.05,.06,.07/
000115 DATA (PTAB(I,1,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
000116 11.,2.,5.,10.,20.,90./
000117 DATA (WTAB(I,2,5),I=1,15)/.001,.002,.003,.004,.009,.012,.018,
000118 1.025,.038,.048,.06,.078,.09,.102,.118/

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C

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000119 DATA (PTAB(I,2,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
000120 11.,2.,5.,10.,20.,50./
000121 DATA (WTAB(I,3,5),I=1,15)/.007,.01,.015,.02,.026,.036,.046,.098,
000122 1.075,.09,.104,.124,.14,.153,.17/
000123 DATA (PTAB(I,3,5),I=1,15)/.001,.002,.005,.01,.02,.05,.1,.2,.5,
000124 11.,2.,5.,10.,20.,50./
000125 DATA (WTAB(I,4,5),I=1,15)/.049,.052,.054,.059,.067,.083,.096,
000126 1.116,.132,.152,.164,.180,.196,.208,.225/
000127 DATA (PTAB(I,4,5),I=1,15)/.001,.003,.005,.01,.02,.05,.09,.2,
000128 1.35,.72,1.013,2.22,4.65,8.5,20./
000129 DATA (WTAB(I,5,5),I=1,15)/.068,.072,.078,.090,.105,.124,.14,
000130 1.156,.165,.182,.196,.209,.224,.24,.256/
000131 DATA (PTAB(I,5,5),I=1,15)/.001,.003,.005,.01,.02,.05,.1,.2,.3,
000132 1.6,1.1,2.0,4.0,9.0,19./
000133 DATA (WTAB(I,6,5),I=1,15)/.108,.112,.13,.144,.158,.172,
000134 1.186,.198,.213,.224,.236,.252,.268,.28,.30/
000135 DATA (PTAB(I,6,5),I=1,15)/.001,.002,.005,.01,.02,.04,.08,.15,.3,
000136 1.5,.85,1.7,3.5,6.2,20./
000137
000138 DATA NT(6)/3/
000139 DATA (TTAB(J,6),J=1,3)/120., 68., 32./
000140 DATA (PTAB(I,1,6),I=1,15) / 15., 20.,30.,40.,60.,80.,100.,125.,150,
000141 1,200., 250.,350.,450.,600.,750./
000142 DATA (PTAB(I,2,6),I=1,15) / 15., 20.,30.,40.,60.,80.,100.,125.,150,
000143 1,200., 250.,350.,450.,600.,750./
000144 DATA (PTAB(I,3,6),I=1,15) / 15., 20.,30.,40.,60.,80.,100.,125.,150,
000145 1,200., 250.,350.,450.,600.,750./
000146 DATA (WTAB(I,1,6),I=1,15)/.0005,.0006,.0007,.0009,.00116,.00137,
000147 1.00155,.00178,.00205,.00250,.0031,.00435,.00565,.0073,.0087/
000148 DATA (WTAB(I,2,6),I=1,15)/.0007,.00078,.00102,.00126,.00173,
000149 1.00207,.0025,.0030,.00348,.0044,.0052,.0068,.0083,.0103,.0122/
000150 DATA (WTAB(I,3,6),I=1,15)/
000151 1.0012,.0014,.0019,.0023,.0030,.0037,.00435,.0052,.00602,
000152 2.0075,.0087,.01138,.0137,.0167,.0197/
000153 DATA NT(7)/2/
000154 DATA (TTAB(J,7),J=1,2)/70., 32./
000155 DATA (PTAB(I,1, 7),I=1,15)/
000156 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000157 2./
000158 DATA (PTAB(I,2, 7),I=1,15)/
000159 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000160 2./
000161 DATA (WTAB(I,1,7),I=1,15)/
000162 1.0002,.00025,.0003,.00043,.0005,.00065,.00082,.00105,.00125,.00146
000163 2,.00186,.00264,.0034,.0044,.00555/
000164 DATA (WTAB(I,2,7),I=1,15)/
000165 1.0002,.00025,.0003,.00044,.00056,.00073,.00096,.00122,.00148,
000166 2.00173,.00224,.00337,.00447,.00585,.0074/
000167 DATA NT(8)/3/
000168 DATA (TTAB(J,8),J=1,3)/120.,72.,32./
000169 DATA (PTAB(I,1, 8),I=1,15)/
000170 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000171 2./
000172 DATA (PTAB(I,2, 8),I=1,15)/
000173 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000174 2./
000175 DATA (PTAB(I,3, 8),I=1,15)/
000176 110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000177 2./
000178 DATA (WTAB(I,1,8),I=1,15)/

```

C



```

000179      1.0001,.0002,.0003,.0004,.0005,.0006,.00075,.0008,.001,.00115,
000180      2.0014,.002,.00255,.0035,.0047/
000181      DATA (WTAB(I,2,6),I=1,15)/
000182      1.00035,.0004,.00045,.0005,.0006,.0009,.0012,.00155,.0018,.0022,
000183      2.0028,.004,.0052,.0066,.0084/
000184      DATA (WTAB(I,3,8),I=1,15)/
000185      1.00065,.0007,.00085,.001,.0012,.0014,.0017,.0024,
000186      2.0032,.0038,.0050,.0069,.0085,.0108,.0144/
000187      DATA NT(9)/3/
000188      DATA (TTAB(J,9),J=1,3)/120.,72.,32./
000189      DATA (PTAB(I,1, 9),I=1,15)/
000190      110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000191      2./
000192      DATA (PTAB(I,2, 9),I=1,15)/
000193      110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000194      2./
000195      DATA (PTAB(I,3, 9),I=1,15)/
000196      110.,15.,20.,30.,40.,55.,75.,100.,125.,150.,200.,300.,400.,550.,750
000197      2./
000198      DATA (WTAB(I,1,9),I=1,15)/
000199      1.0001,.00013,.00017,.0002,.00025,.0003,.00037,.00048,.00058,
000200      2.00067,.00087,.00122,.00163,.00221,.00291/
000201      DATA (WTAB(I,2,9),I=1,15)/
000202      1.0002,.00023,.00026,.00036,.00045,.00058,.0007,.00085,
000203      2.00099,.00111,.00136,.0019,.0024,.00312,.00396/
000204      DATA (WTAB(I,3,9),I=1,15)/
000205      1.00025,.00034,.00042,.00055,.00067,.00082,.001,.00122,
000206      2.00144,.00163,.00199,.00264,.00328,.0043,.00578/
000207
000208      C
000209      IF (W .LE. 0.) W= 1.E-20
000210      IF(JACK .GT. 0) GO TO 102
000211      DO 105 K=1,25
000212      IF (NT(K) .EQ. 0) GO TO 90
000213      NTI=NT(K)
000214      DO 101 J=1,NTI
000215      TTAB(J,K)=1./(TTAB(J,K)+460.)
000216      DO 101 I=1,15
000217      WTAB(I,J,K)=ALOG(WTAB(I,J,K))
000218      PTAB(I,J,K)=ALOG(PTAB(I,J,K))
000219      101 CONTINUE
000220      90 CONTINUE
000221      105 CONTINUE
000222      102 CONTINUE
000223      IS=IDSMTX(IDSORB,ID)
000224      IF(IS.EQ.0) GO TO 999
000225      JACK = JACK + 1
000226      RT=1./(T+460.)
000227      GO TO (201,202), KPW
000228      201 WL=ALOG(W)
000229      N=NT(IS)
000230      PKEQ1=XYZMAP(1,WTAB(1,1,IS), PTAB(1,1,IS),15,TTAB(1,IS),N ,2,2,WL,
000231      ,1RT,ANS)
000232      P =EXP(PKEQ1)
000233      IF (PKEQ .LT. 0.0) PKEQ=0.0
000234      RETURN
000235      202 PL=ALOG(P)
000236      N=NT(IS)
000237      W01=XYZMAP(1,PTAB(1,1,IS),WTAB(1,1,IS),15,TTAB(1,IS),N,2,2,PL,RT,
000238      1ANS)
000239      W=EXP(W01)
000240      RETURN
000241      999 WRITE(6,998) IDSORB,ID
000242      998 FORMAT(///// ' EQUILIBRIUM DATA UNAVAILABLE FOR'/' IDSORB ='I4'/
000243      1 ID =' I4)
000244      CALL EXIT
000245      END

```

* ELT FCOAD,1,710712, 56800 , 1

```

000001      FUNCTION FCOAD(IDSORB,H2O)
000002      C
000003      C
000004      DIMENSION H2OT(12), FCOADT(12,5)
000005      DATA H2OT/ 0.00, .01, .02, .03, .04, .05, .06, .07, .08, .10,
000006      1.12, .60/
000007      DATA (FCOADT(I,1),I=1,12)/1.,.98,.88,.72,.575, .436, .313, .22,
000008      1.155, .086, .055, .0/
000009      DATA(FCOADT(I,3),I=1,12)/1., .794, .63, .503, .415, .35, .298,
000010      1.252, .214, .148, .085, .0/
000011      CALL LAGIN2(606, H2OT          ,12,2,H2O,FCOAD,FCOADT(1,IDSORB))
000012      RETURN
000013      END

```

* ELT FDEQID,1,710514, 38495 , 1

```

000001      SUBROUTINE FDEQID(C1,C2,C3,D,VAR,NN)
000002      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
000003      DOUBLE PRECISION C1,C2,C3,D,VAR,B,Q
000004      NN1=NN-1
000005      B(1)=C3(1)/C2(1)
000006      DO 41 J=2,NN1
000007      41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000008      Q(1)=D(1)/C2(1)
000009      DO 42 J=2,NN
000010      42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
000011      VAR(NN)=Q(NN)
000012      DO 43 J=2,NN
000013      L=NN+1-J
000014      43 VAR(L)=Q(L)-B(L)*VAR(L+1)
000015      RETURN
000016      END

```

* ELT FDEQIM,1,710514, 38492 , 1

```

000001      SUBROUTINE FDEQIM(C1,C2,C3,D,VAR,NN)
000002      DIMENSION C1(1),C2(1),C3(1),D(1),VAR(1),B(41),Q(41)
000003      NN1=NN-1
000004      B(1)=C3(1)/C2(1)
000005      DO 41 J=2,NN1
000006      41 B(J)=C3(J)/(C2(J)-C1(J)*B(J-1))
000007      Q(1)=D(1)/C2(1)
000008      DO 42 J=2,NN
000009      42 Q(J)=(D(J)-C1(J)*Q(J-1))/(C2(J)-C1(J)*B(J-1))
000010      VAR(NN)=Q(NN)
000011      DO 43 J=2,NN
000012      L=NN+1-J
000013      43 VAR(L)=Q(L)-B(L)*VAR(L+1)
000014      RETURN
000015      END

```



© ELT FLAP,1,710719, 62342 , 1

```

000001      SUBROUTINE FLAP
000002      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,          PK (2,20),PC02I ,TS (20)
000003      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000004      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,
000005      3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000006      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000008      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000010      8          HXG(20),HXS(20),HXC(20),HSG(20),
000011      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTC02,TOTH20,
000012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX;
000013      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VC02A,SABCO2,TC02A,
000014      1RS1(20,9),          A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000017      3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000018      4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000019      5          WM(2),TIME,CYCLE,DT0, DTMAX,WI,TI,PC02C,
000020      6VOLCAB,RC02C,
000021      7NCYCLT,NPRINT,NCYCLE,NDTC0N,NTEMP,NSTART,NPR,DT,DTT(4),SABCO5
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000023      1          CP1,CP2,X, C1P,C2P,C3P,D1P
000024      DIMENSION DUMMY(20),DUMM1(20),IDUMMY(20)
000025      NAMELIST /CHECK/
000026      1TG,PH2OI,TGI,PA,PK,PC02I,TS,TC,TX,TS1,TS2,TX1,TX2,TC1,TC2,W,PT,
000027      2GMR,GMW,ABED,AVC,ASG,ASX,AGX,AXC, AVX,RHOG,RHOSB,RHOS,RHOC,RHOX,CP
000028      3G, CPC,CPX,CPS,DX,POUT,TIMET,WTACMS,WTSG,PUMP,NPSET,NDR4,
000029      4NDXMAC,NBCOUT,NDX1,NDXM,NOG,HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK,UC,T2
000030      568, TOTC02,TOTH20,SUMPTM,AVMSL1,AVSGL1,HTR,TMAX,A,F,C,VS,DVS,DVS1
000031      CALL FLIP(W,TG,TS,TX,TC,NDX1,NDR4,NOG,UC)
000032      CALL FLCP(ABED,AVC,ASG,ASX,AGX,NDX1)
000033      CALL FLOP(AXC,AVX,RHOG,RHOSB,RHOC,NDX1)
000034      CALL FLOP(RHOX,CPG,CPC,CPX,CPS,NDX1)
000035      CALL FLOP(HXG,HXS,HXC,HSG,DH,NDX1)
000036      CALL FLOP(DIF,GK,PT ,X ,HTR ,NDX1)
000037      CALL FLOP (TS1,DUMMY,DUMMY,DUMMY,DUMMY,NDX1)
000038      CALL FLOP(TS2,TX1,TX2,TC1,TC2,NDX1)
000039      NDX2=NDX1+1
000040      CALL FLOP(SK,TKX,DUMMY,DUMMY,DUMMY,NDX2)
000041      DO 61 K=1,2
000042      DO 62 N=1, NDX1
000043      DUMM1(N)=FR(K,N)
000044      62 DUMMY(N)=PK(K,N)
000045      DO 61 N=1,NDX1
000046      I=NDX1+1-N
000047      FR(K,I)=DUMM1(N)
000048      61 PK(K,I)=DUMMY(N)
000049      DO 63 N=1,NDX1
000050      63 IDUMMY(N)=IDSORB(N)
000051      DO 64 N=1,NDX1
000052      I=NDX1+1-N
000053      64 IDSORB(I)=IDUMMY(N)
000054      RETURN
000055      END

```




```

000001      SUBROUTINE FLIP(W,TG,TS,IX,TC,NX,NR,NOG,UC)
000002      C      THIS SUBROUTINE INVERTS BED LOADINGS AND TEMPERATURES
000003      DIMENSION W( 4,20),TG(20),TS(20),TX(20),TC(20),UC(20)
000004      DIMENSION TW( 4,20),TTG(20),TTS(20),TTX(20),TTC(20),TUC(20)
000005      DO 5 I=1,NX
000006      DO 6 J=1,NR
000007      6 TW(J,I)=W(J,I)
000008      TTC(I)=TC(I)
000009      TTG(I)=TG(I)
000010      TTS(I)=TS(I)
000011      TTX(I)=TX(I)
000012      5 TUC(I)=UC(I)
000013      DO 10 N=1,NX
000014      I=NX+1-N
000015      DO 15 J=1,NR
000016      15 W(J,I)=TW(J,N)
000017      TG(I)=TTG(N)
000018      TS(I)=TTS(N)
000019      TX(I)=TTX(N)
000020      TC(I)=TTC(N)
000021      10 UC(I)=-TUC(N)
000022      NOG=NX+1-NOG
000023      RETURN
000024      END
    
```

```

000001      SUBROUTINE FLOP(A,B,C,D,E,NX)
000002      DIMENSION A(41),B(41),C(41),D(41),E(41)
000003      DIMENSION AA(20),BB(20),CC(20),DD(20),EE(20)
000004      DO 10 I=1,NX
000005      AA(I)=A(I)
000006      BB(I)=B(I)
000007      CC(I)=C(I)
000008      DD(I)=D(I)
000009      10 EE(I)=E(I)
000010      DO 20 N=1,NX
000011      I=NX+1-N
000012      A(I)=AA(N)
000013      B(I)=BB(N)
000014      C(I)=CC(N)
000015      D(I)=DD(N)
000016      20 E(I)=EE(N)
000017      RETURN
000018      END
    
```

```

000001      SUBROUTINE GAST (DX,RHOG,CPG,U,TS,IX,NDX1,ASG,HSG,AXG,HXG,TG,VOIDF
000002      1)
000003      DIMENSION RHOG(1),CPG(1),U(1),TS(1),TX(1),TG(1),ASG(1),HSG(1),HXG(
000004      11),VOIDF(1),AXG(1)
000005      W=1.0
000006      N2= NDX1-1
000007      TG(1)=TS(1)
000008      DO 10 N= 1, N2
000009      F= 0.5*(VOIDF(N)+ VOIDF(N+1))
000010      AS1=ASG(N+1)
000011      HS1=HSG(N+1)
000012      AX1=AXG(N+1)
000013      HX1=HXG(N+1)
000014      CP1=CPG(N)
000015      RO = 0.5*(RHOG(N)+RHOG(N+1))
000016      U1= 0.5*( U(N)+U(N+1))
000017      TS1=TS(N+1)
000018      TX1=TX(N+1)
000019      C1=1./(F*RO*CP1*U1)
000020      D=C1*(AS1*HS1*TS1+AX1*HX1*TX1)
000021      A=(AS1*HS1+AX1*HX1)*C1
000022      10 TG(N+1)=((1./DX-A*(1.-W))*TG(N)+D)/(1./DX+A*W)
000023      RETURN
000024      END
    
```



* ELT GASTA.1,710514, 38501 , 1

```

000001      SUBROUTINE GASTA(GMR,CPG,ABED,NDX1,TG1,ASG,HSG,AXG,HXG,DX,TG,TS,TX
000002      1)
000003      C
000004      C      GAS TEMPERATURE CALCULATIONS FOR ADSORPTION
000005      C
000006      DIMENSION CPG(1),ASG(1),HSG(1),HXG(1),TG(1),TS(1),TX(1),ABED(1),
000007      1AXG(1)
000008      C
000009      TG(NDX1+1) = TG1
000010      DO 10 N=1,NDX1
000011      C=GMR*CPG(N)/ABED(N)
000012      N1=NDX1+1-N
000013      C1=ASG(N1)*HSG(N1)+AXG(N1)*HXG(N1)
000014      10 TG(N1) = (TG(N1+1)/DX+(ASG(N1)*HSG(N1)*TS(N1)+AXG(N1)
000015      1                                     *HXG(N1)*TX(N1))/
000016      1C)/(1./DX+C1/C)
000017      RETURN
000018      END
    
```

* ELT HXCORE.1,710719, 62343 , 1

```

000001      SUBROUTINE HXCORE
000002      COMMON/AD/ TG(20),PH201 ,TGI ,PA ,          PK (2,20),PCO2I ,TS (20)
000003      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000004      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,PO2,
000005      3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000006      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000008      6POUT(10),TIMET(10),WTACMS,WTSC ,PUMP(10),VPUMP(10),CPP(20),
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000010      8          HXG(20),HXS(20),HXC(20),HSG(20),
000011      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH2O,
000012      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000013      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VC02A,SABC02, TCO2A,
000014      1RS1(20,9),          A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000017      3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000018      4(20,4),          C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000019      5          WM(2),TIME,CYCLE,DT0,          DTMAX,WI,TI,PCO2C,
000020      6VOLCAB,RCO2C,
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SARCOS
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000023      1          CP1,CP2,X,          C1P,C2P,C3P,D1P
000024      EQUIVALENCE (NDX,NDX1)
000025      DIMENSION S1(20),S2(20),S3(20),DD(20)
000026      C
000027      DN=DT+DT0
000028      DO 10 N=1,NDX
000029      T1= AVX(N)*(HXC(N)+HXS(N)+HXG(N))*0.5
000030      S1(N)=-TKX(N)/DX/DX
000031      S3(N)= -TKX(N+1)/DX/DX
000032      S2(N)= RHOX(N)*CPX(N)/DN -S1(N) - S3(N) + T1
000033      10 DD(N) = RHOX(N)*CPX(N)/DN*TX2(N) + AVX(N)*(HXC(N)
000034      1*TC1(N) + HXS(N)*TS1(N)+HXG(N)*TG(N)) - T1*TX2(N)+HTR(N)/(ABED(N)*
000035      2ASX(N)/AVX(N)*DX)
000036      S2(1)=S2(1)+S1(1)
000037      S1(1)=0.
000038      S2(NDX)=S2(NDX)+S3(NDX)
000039      S3(NDX)=0.0
000040      CALL FDEQIM(S1,S2,S3,DD,TX,NDX)
000041      RETURN
000042      END
    
```

* ELT IFN.1,710514, 38502 , 1

```

000001      FUNCTION IFN(N,NDXM)
000002      IFN=1
000003      IF(N.GT.NDXM)IFN=2
000004      RETURN
000005      END
000006      C
    
```



* ELT LAGIN2,1,710514, 38503 , 1

```

000001      SUBROUTINE LAGIN2(ID,X,NP,ND,XO,YO,Y)
000002      C      REVISED FOR FORTRAN IV 8-8-65 S. WONG
000003      C      DIMENSION X(2), Y(2)
000004      C
000005          ILO=1
000006          IF(XO-X(1))10,16,4
000007      4  IF(XO-X(NP))19,13,7
000008      7  ILO=NP-1
000009      10  IHI=ILO+1
000010          GO TO 46
000011      13  ILO=NP
000012      16  YO=Y(ILO)
000013          RETURN
000014      19  DO 22 ILO=2,NP
000015          IF(XO-X(ILO))25,16,22
000016      22  CONTINUE
000017      25  IHI=ILO
000018          ILO=IHI-1
000019          IF(ND-2)46,46,28
000020      28  DO 43 I=3,ND
000021          IF(ILO-1)40,40,31
000022      31  IF(IHI-NP)34,37,37
000023      34  IF (2.*XO-X(ILO-1)-X(IHI+1)) 37,37,40
000024      37  ILO=ILO-1
000025          GO TO 43
000026      40  IHI=IHI+1
000027      43  CONTINUE
000028      46  YO=0.0
000029          PN=1.0
000030          DO 49 I=ILO,IHI
000031      49  PN=PN*(XO-X(I))
000032          DO 58 I=ILO,IHI
000033          P=PN/(XO-X(I))
000034          DO 55 J=ILO,IHI
000035          IF(J-1)52,55,52
000036      52  P=P/(X(I)-X(J))
000037      55  CONTINUE
000038          YO=YO+P*Y(I)
000039      58  CONTINUE
000040          RETURN
000041      1  FORMAT (97X,7HLAGIN2 ,14,E12.5)
000042          END

```



@ ELT MAIN4B.1.710719. 62345 , 1

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000001      C MAIN PROGRAM FOR ANALYZING 4-BED SYSTEM FOR CO2 RECOVERY
000002      C
000003      COMMON/AD/ TG(20),PH201 ,TGI ,PA ,      PK (2,20),PCO2I ,TS (20) *NEW
000004      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20), *NEW
000005      2TC2 (20),W (4,20),PT (20),      GMR ,GMW,GVIS, PN2,P02, *NEW
000006      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20), *NEW
000007      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20), *NEW
000008      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20), *NEW
000009      6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20), *NEW
000010      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORR(20), *NEW
000011      8      HXG(20),HXS(20),HXC(20),HSG(20), *NEW
000012      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20, *NEW
000013      1SUMPTN,AVHSL1,AVSGL1,HTR(20),TMAX, *NEW
000014      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2, TCO2A, *NEW
000015      1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20), *NEW
000016      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20), *NEW
000017      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20), *NEW
000018      3FR(2,20),      P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3 *NEW
000019      4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20), *NEW
000020      5      WM(2),TIME,CYCLE,DT0,      DTMAX,W1,TI,PCO2C, *NEW
000021      6VOLCAB,RCO2C, *NEW
000022      7NCYCLT,NPRINT,NCYCLE,NOTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS *NEW
000023      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B, *NEW
000024      1      CP1,CP2,X,      C1P,C2P,C3P,D1P *NEW
000025      COMMON TG1(20),PH2011,TGI1,PA1,      PK1(2,20),PCO2I1 ,TS01(20) **-1
000026      1,TC01(20),TX01(20), TS11(20),TS21(20),TX11(20),TX21(20),TC11(20),
000027      2TC21(20),W1(4,20),PT1(20),      GMR1,GMW1,GVIS1,PN21,P021
000028      COMMON TG2(20),PH2012,TGI2,PA2,      PK2(2,20),PCO2I2 ,TS02(20)
000029      1,TC02(20),TX02(20), TS12(20),TS22(20),TX12(20),TX22(20),TC12(20),
000030      2TC22(20),W2(4,20),PT2(20),      GMR2,GMW2,GVIS2,PN22,P022
000031      COMMON TG3(20),PH2013,TGI3,PA3,      PK3(2,20),PCO2I3 ,TS03(20)
000032      1,TC03(20),TX03(20), TS13(20),TS23(20),TX13(20),TX23(20),TC13(20),
000033      2TC23(20),W3(4,20),PT3(20),      GMR3,GMW3,GVIS3,PN23,P023
000034      COMMON TG4(20),PH2014,TGI4,PA4,      PK4(2,20),PCO2I4 ,TS04(20)
000035      1,TC04(20),TX04(20), TS14(20),TS24(20),TX14(20),TX24(20),TC14(20),
000036      2TC24(20),W4(4,20),PT4(20),      GMR4,GMW4,GVIS4,PN24,P024
000037      COMMON/B1/ RDB(405),IDB(29)
000038      COMMON/B2/RMB(405),IMB(29)
000039      COMMON/B1A/RDBA(260)
000040      COMMON/B1D/RDBD(260)
000041      COMMON/B2A/ RMB A(260)
000042      COMMON/B2D/ RMB D(260)
000043      DIMENSION RB1M(349),RB2M(349),RB3M(349),RB4M(349),RMAIN(11),
000044      1IMAIN(06),KBED(4)
000045      EQUIVALENCE (RB1M(1),TG1(1)),(RB2M(1),TG2(1)),(RB3M(1),TG3(1)),
000046      1(RB4M(1),TG4(1)),(RMAIN(1),WM(1)),(IMAIN(1),NCYCLT)
000047      NAMELIST/MAIN/ WM, CYCLE,DTMAX,W1,TI,PCO2C,VOLCAB,RCO2C,
000048      1NPRINT,NOTCON,NTEMP,      TGC,PAC,PH20C,TGHX
000049      2,PCO2A,VCO2A,SABCO2,TCO2A,KBED,TIMEDS, NCT1, NST1, NCT2, NST2
000050      NAMELIST/B1M/      PA1,      TS01,TC01,TX01,W1,
000051      1GMR1,GMW1,      PN21,P021
000052      NAMELIST/B2M/      PA2,      TS02,TC02,TX02,W2,
000053      1GMR2,GMW2,      PN22,P022
000054      NAMELIST/B3M/      PA3,      TS03,TC03,TX03,W3,
000055      1GMR3,GMW3,      PN23,P023
000056      NAMELIST/B4M/      PA4,      TS04,TC04,TX04,W4,
000057      1GMR4,GMW4,      PN24,P024
000058      DATA PT2,PT4/ 40*3.0/,X/20*1./,C/20*0.2E-3/

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000059      DATA DTT/4*1./
000060      1 CONTINUE      * TO READ IN DATA FOR A NEW PROBLEM
000061      108 FORMAT(13A6,A2)
000062      109 FORMAT(20X,13A6,A2)
000063      READ(5,MAIN)
000064      WRITE(6,MAIN)
000065      READ(5,B1M)
000066      WRITE(6,B1M)
000067      READ(5,B2M)
000068      WRITE(6,B2M)
000069      READ(5,B3M)
000070      WRITE(6,B3M)
000071      READ(5,B4M)
000072      WRITE(6,B4M)
000073      CALL READ1
000074      CALL READ2
000075      CALL READ3
000076      CALL READ4
000077      SABCOS=SABC02
000078      NHALF=1
000079      DO 102 N= 1, 20
000080      TC11(N)=TC01(N)
000081      TC21(N)=TC01(N)
000082      TX11(N)=TX01(N)
000083      TX21(N)=TX01(N)
000084      TS11(N)=TS01(N)
000085      TS21(N)=TS01(N)
000086      TC12(N)=TC02(N)
000087      TC22(N)=TC02(N)
000088      TX12(N)=TX02(N)
000089      TX22(N)=TX02(N)
000090      TS12(N)=TS02(N)
000091      TS22(N)=TS02(N)
000092      TC13(N)=TC03(N)
000093      TC23(N)=TC03(N)
000094      TX13(N)=TX03(N)
000095      TX23(N)=TX03(N)
000096      TS13(N)=TS03(N)
000097      TS23(N)=TS03(N)
000098      TC14(N)=TC04(N)
000099      TC24(N)=TC04(N)
000100      TX14(N)=TX04(N)
000101      TX24(N)=TX04(N)
000102      TS14(N)=TS04(N)
000103      TS24(N)=TS04(N)
000104      102 CONTINUE
000105      NCYCLT=NCT1
000106      NSTART=NST1
000107      ASSIGN 103 TO NSUB48
000108      GO TO 104
000109      103 CONTINUE
000110      CALL BED4(1,0,3,RB1M,RDR,IDB,RDBA,ISTOPC,KBED)
000111      CALL BED4(2,0,3,RB2M,RMS,IMB,RMBA,ISTOPC,KBED)
000112      DO 201 K=1,60
000113      N=K+120
000114      RMBD(N)=RMBA(N)
000115      RDBD(N)=RDBA(N)
000116      201 CONTINUE
000117      NCYCLT=NCT2
000118      NSTART=NST2

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000119          ASSIGN 105 TO NSUB4B
000120          GO TO 104
000121          105 CONTINUE
000122          CALL EXIT
000123          C
000124          C
000125          104 CONTINUE
000126          C  START SUB4B
000127          NCYCLE=1
000128          101 CONTINUE
000129          IF(NCYCLE .GT. NCYCLT) GO TO NSUB4B
000130          TIME = 0.0
000131          DTO = 0.0
000132          DT=1.E-5
000133          NPR = 1
000134          GO TO 3
000135          4 CONTINUE
000136          GO TO ( 3,42),NDTCN
000137          42 DT=DTMAX/10.0
000138          IF(TIME .LT. 1.E-4) DT=DTMAX/1000.0
000139          IF(TIME .GT. 0.06) DT=DTMAX
000140          GO TO 5
000141          3 CONTINUE
000142          DT=AMIN1(DTT(1),DTT(2),DTT(3),DTT(4))
000143          IF(TIME .LT. 8.E-5) DT=1.E-5
000144          5 IF((TIME+DT) .GT. CYCLE) DT = CYCLE-TIME
000145          TIME=TIME+DT
000146          GO TO(20,21), NHALF
000147          C *****PART TO BE CHANGED FOR DIFFERENT HOOK-UP OF SYSTEM *****
000148          C  FIRST HALF CYCLE
000149          20 CONTINUE
000150          PC02I1=PC02C
000151          PH20I1=PH20C
000152          TG11=TC
000153          ISTOPC=0
000154          CALL BED4(1,0,1,RB1M,RDB,IDB,ROBA,ISTOPC,KBED)
000155          PC02I2=PK (1,1)
000156          PH20I2=PK (2,1)
000157          TG12=TC (1)
000158          IF(TG1(1) .GT. TGHX) TG12=TGHX
000159          RMBA(201)=TC01(10)
000160          35 CALL BED4(2,0,1,RB2M,RMB,IMB,RMBA,ISTOPC,KBED)
000161          DPC02C=DT*(RC02C-GMR*(PC02C-PK2(1,1))*44./ (PA*GMW))*554.*530./
000162          1(44.*VOLCAB)
000163          IF((KBED(1).EQ.0),AND.(KBED(2).EQ.0))DPC02C=0.
000164          PC02C=PC02C+DPC02C
000165          PC02I3=PK (1,1)
000166          PH20I3=0.00000
000167          TG13=TC (1)
000168          IF(TIME.GT.TIMEDS) ISTOPC=1
000169          CALL BED4(3,1,1,RB3M,RDB,IDB,ROBD,ISTOPC,KBED)
000170          RMBD(201)=TC03(10)
000171          CALL BED4(4,0,2,RB4M,RMB,IMB,RMBD,ISTOPC,KBED)
000172          C ***** TO BE CHANGED UP TO HERE *****
000173          NPR = NPR+1
000174          DTO=DT
000175          IF(TIME .GE. CYCLE) NHALF=2
000176          IF(TIME .GE. CYCLE) GO TO 101
000177          GO TO 4
000178          C *****PART TO BE CHANGED FOR DIFFERENT HOOK-UP OF SYSTEM *****

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000179      C SECOND HALF CYCLE
000180      21 CONTINUE
000181          ISTOPC=0
000182          PC0213=PC02C
000183          PH2013=PH20C
000184          TG13=TCG
000185          CALL BED4(3,0,1,RB3M,RDB,IDB,RDRA,ISTOPC,KBED)
000186          PC0214=PK (1,1)
000187          PH2014=PK (2,1)
000188          TG14=TCG (1)
000189          IF(TG3(1) .GT. TGHX) TG14=TCGX
000190          RMBA(201)=TC03(10)
000191      36 CALL BED4(4,0,1,RB4M,RMB,IMB,RMBA,ISTOPC,KBED)
000192          DPC02C=DT*(RC02C-GMR*(PC02C-PK4(1,1))*44./ (PA*GMW))*554.*530./
000193          1(44.*VOLCAB)
000194          IF((KBED(3).EQ.0),AND.(KBED(4).EQ.0))DPC02C=0.
000195          PC02C=PC02C+DPC02C
000196          PC0211=PK (1,1)
000197          PH2011=0.0000
000198          TG11=TCG (1)
000199          IF(TIME.GT.TIMEDS) ISTOPC=1
000200          CALL BED4(1,1,1,RB1M,RDB,IDB,RDBD,ISTOPC,KBED)
000201          RMBD(201)=TC01(10)
000202          CALL BED4(2,0,2,RB2M,RMB,IMB,RMBD,ISTOPC,KBED)
000203      C ***** TO BE CHANGED UP TO HERE *****
000204          NPR = NPR+1
000205          DT0=DT
000206          IF(TIME .GE. CYCLE) NHALF=1
000207          IF(TIME .GE. CYCLE) NCYCLE=NCYCLE+1
000208          IF(TIME .GE. CYCLE) GO TO 101
000209          GO TO 4
000210          END

```



© ELT NEWT02,1,710609, 32711 , 1

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030001      SUBROUTINE NEWT02(N1,NGO,X,Y,X0,Y0,XMIN,XMAX,ER)
000002      C   SET N1=1 IN MAIN PROGRAM BEFORE CALL NEWTON. THE ROUTINE
000003      C   FINDS X FOR Y=0 GIVES NGO=1 IF RECALCULATIONS REQUIRED.
000004      C   GIVES NGO=2 IF CONVERGENCE REACHED.
000005      N1=N1-1
000006      IF( ABS(Y)-ER) 8,8,5
000007      5 IF(N1)7,6,7
000008      6 Y0=Y
000009      X0=X
000010      X=X0+(XMAX-XMIN)*0.01
000011      IF(X-XMAX)21,21,14
000012      14 X=X0-(XMAX-XMIN)*0.01
000013      GO TO 21
000014      7 SLOPE=(Y-Y0)/(X-X0)
000015      Y0=Y
000016      X0=X
000017      X=X-Y/SLOPE
000018      IF(N1+8)20,20,21
000019      20 X=0.5*(X+X0)
000020      IF(N1+20)22,22,21
000021      22 WRITE (6,23)
000022      WRITE (6,30) X,Y,X0,Y0,ER
000023      23 FORMAT (32H0EXCEED 20 ITERATIONS IN NEWTON //)
000024      N1=0
000025      ER=5.*ER
000026      21 CONTINUE
000027      IF(X-XMIN)11,11,12
000028      11 X=XMIN
000029      IF(X-X0)9,8,9
000030      12 IF(X-XMAX)9,13,13
000031      13 X=XMAX
000032      IF(X-X0)9,8,9
000033      9  NGO=1
000034      RETURN
000035      8  NGO=2
000036      N1=1
000037      RETURN
000038      30 FORMAT(14H X,Y,X0,Y0,ER= 5G14.4)
000039      END

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* ELT PRADSB,1,710719, 62347 , 1

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000001          SUBROUTINE PRADSB(IBED)
000002      C
000003          COMMON/AD/ TG(20),PH201 ,TGI ,PA ,          PK (2,20),PCO21 ,TS (20)
000004          1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000005          2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,
000006          3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000007          4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000008          5PCPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000009          6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000010          7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORR(20),
000011          8          HXG(20),HXS(20),HXC(20),HSG(20),
000012          9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,
000013          1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000014          1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VC02A,SABC02, TC02A,
000015          1RS1(20,9),          A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000016          1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000017          2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000018          3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000019          4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000020          5          WM(2),TIME,CYCLE,DT0,          DTMAX,WI,TI,PCO2C,
000021          6VOLCAB,RCO2C,
000022          7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS
000023          DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,R,
000024          1          CP1,CP2,X,          C1P,C2P,C3P,D1P
000025      C
000026          DIMENSION AVLD(41)
000027          EQUIVALENCE(NDX,NDX1)
000028          AVMSLD=0.0
000029          AVSGLD=0.0
000030          AVRCO2=0.0
000031          AVRH20=0.0
000032          AVPH20 = SUMPTM/TIME
000033          AVH2OP=GMR*AVPH20*18./((PA*GMW)
000034      C
000035          TIMEM=60.*TIME
000036          WRITE(6,499)IBED
000037          WRITE(6,100) NCYCLE,TIME ,TIMEM,DT
000038          WRITE (6,101)
000039          WRITE(6,102)(N,PK(1,N),PK(2,N),
000040          1          TG(N),TS(N),TC(N),TX(N),N=1,NDX)
000041          WRITE(6,103)PK(1,NDX1+1),PK(2,NDX1+1),TG(NDX1+1)
000042          103 FORMAT('          INLET' F10.4,F12.4,F19.4)
000043          WRITE (6,202)
000044          N1=NDXM+1
000045          NDR3=NDR4-1
000046          DO 20 N= 1, NDXM
000047          SUMMS=0.0
000048          SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000049          IF(NDR4.EQ.2) AVLD(N) = SUMMS
000050          IF(NDR4.EQ.2) GO TO 20
000051          DO 22 NR=2,NDR3
000052          22 SUMMS=SUMMS+W(NR,N)
000053          AVLD(N)=SUMMS/NDR3
000054          20 CONTINUE
000055          DO 30 N= N1,NDX1
000056          SUMMS=0.0
000057          SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000058          IF(NDR4.EQ.2) AVLD(N) = SUMMS

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000059      IF(NDR4.EQ.2) GO TO 30
000060      DO 33 NR=2, NDR3
000061      33 SUMMS=SUMMS+W(NR,N)
000062      AVLD(N)=SUMMS/NDR3
000063      30 CONTINUE
000064      SUM=0.
000065      IF(NDXMAC .EQ. 0) GO TO 35
000066      DO 31 N= 1, NDXMAC
000067      31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000068      AVMSLD = SUM/WTACMS
000069      SUM=0.
000070      35 CONTINUE
000071      IF((NDX1-NDXM) .EQ. 0) GO TO 40
000072      DO 32 N= N1,NDX1
000073      32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000074      AVSGLD=SUM/WTSG
000075      40 CONTINUE
000076      DO 10 N=1,NDX
000077      10 WRITE (6,203)N, AVLD(N)
000078      1      ,*(N(NR,N),NR=1,NDR4)
000079      IF(TIME .LT. 1.1E-5) AVMSL1=AVMSLD
000080      IF(TIME .LT. 1.1E-5) AVSGL1=AVSGLD
000081      AVRCO2=WTACMS*(AVMSLD-AVMSL1)/TIME
000082      AVRH2O=WTSG*(AVSGLD-AVSGL1)/TIME
000083
C
000084      DIMENSION F1(9),F2(9),F3(9),F4(9), F5(9),F6(9),F7(9)
000085      WRITE(6,205) F1,AVMSLD,F2,AVSGLD,F3,AVRCO2,F4,AVRH2O,F5,TOTKWH,
000086      F6,TOTHTC,F7,AVPH2O
000087      205 FORMAT(////(9A6,F8.4,6X,9A6,F8.4 ))
000088      DATA F1/' AVG CO2 LOADING IN CO2 SORBENT (LB/LB)'/
000089      DATA F2/' AVG H2O LOADING IN DESICCANT (LB/LB)'/
000090      DATA F3/' TIME AVG CO2 ADSORPTION RATE (LB/HR)'/
000091      DATA F4/' TIME AVG H2O ADSORPTION RATE (LB/HR)'/
000092      DATA F5/' ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)'/
000093      DATA F6/' HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)'/
000094      DATA F7/' TIME AVG OUTLET PH2O (MM)'/
000095
C
000096      RETURN
000097      499 FORMAT(8H1BED NO. I3)
000098      100 FORMAT (1H0,16H ADSORPTION CYCLE I3/
000099      1      3X,5HTIME=,F9.5,1X2HHR,F12.3,1X,3HMIN,
000100      1      5X,15HTIME INCREMENT=F7.5,1X2HHR)
000101      101 FORMAT (//2X,10H AXIAL NODE,3X,7HPCO2,MM,5X,7HPH2O,MM,8X,
000102      1      11HGAS TEMP, F
000103      1      ,8X,15HSORBENT TEMP, F      ,6X,15HCOOLANT TEMP, F      ,7X,15HMX CO
000104      2RE TEMP, F )
000105      102 FORMAT(//19,2F12.4,5X,4(F14.4,6X))
000106      202 FORMAT (// 38H LOADING AT INTERIOR OF SORBENT, LB/LB
000107      1      //4X,4HSORB/4X,4HNOD
000108      1E,3X, 3H AVG, 9X,
000109      1      1H1,9X,1H2,9X,1H3,9X,1H4
000110      2      /6H AXIAL/3H NODE)
000111      203 FORMAT ( 15,4X,12(F6.4,4X))
000112      END

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* ELT PRDES8,1,710719, 62348 , 1

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000011          SUBROUTINE PRDES8( IDED)
000012          C
000013          C
000014          COMMON/AD/ TG(20),PH20I ,TGI ,PA ,          PK (2,20),PC02I ,TS (20)
000015          1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000016          2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,
000017          3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000018          4AVX(20),RHOG(20),RHOS(20),RHOS(20),RHOC(20),RHOX(20),
000019          5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000020          6POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000021          7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000022          8          HXG(20),HXS(20),HXC(20),HSG(20),
000023          9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTC02,TOTH20,
000024          1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000025          1TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VCO2A,SARCO2,TC02A,
000026          1RS1(20,9),          A(20),F(20),C(20),VS(20),DVS1(20),RS(20),
000027          1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000028          2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000029          3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000030          4(20,4),          C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000031          5          WM(2),TIME,CYCLE,DT0,          DTMAX,WI,TI,PC02C,
000032          6VOLCAR,RC02C,
000033          7NCYCLT,NPRINT,NCYCLE,NDTC0N,NTEMP,NSTART,NPR,DT,DTT(4),SARCOS
000034          8DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,G,B,
000035          9          CP1,CP2,X,          C1P,C2P,C3P,D1P
000036          DIMENSION AVLD(41)
000037          EQUIVALENCE(NDX,NDX1)
000038          C
000039          AVMSLD=0.0
000040          AVSGLD=0.0
000041          AVRC02=0.0
000042          AVRH20=0.0
000043          TIMEM=60.*TIME
000044          WRITE(6,499)IBED
000045          WRITE(6,100) NCYCLE,TIME ,TIMEM,DT
000046          WRITE (6,101)
000047          WRITE (6,102)(N,PT(N),TG(N),TS(N),TC(N),TX(N),N=1,NDX)
000048          IF(( NPSET(1) .GT. 0) .OR. (NPSET(2) .GT. 0)) GO TO 99
000049          99 WRITE (6,202)
000050          N1=NDXM+1
000051          NDR3=NDR4-1
000052          DO 20 N= 1, NDXM
000053          SUMMS=0.0
000054          SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000055          IF(NDR4 .EQ. 2) AVLD(N) = SUMMS
000056          IF(NDR4.EQ.2) GO TO 20
000057          DO 22 NR=2,NDR3
000058          22 SUMMS=SUMMS+W(NR,N)
000059          AVLD(N)=SUMMS/NDR3
000060          20 CONTINUE
000061          DO 30 N= N1,NDX1
000062          SUMMS=0.0
000063          SUMMS=SUMMS+0.5*(W(1,N)+W(NDR4,N))
000064          IF(NDR4.EQ.2) AVLD(N) = SUMMS
000065          IF(NDR4.EQ.2) GO TO 30
000066          DO 33 NR=2, NDR3
000067          33 SUMMS=SUMMS+W(NR,N)
000068          AVLD(N)=SUMMS/NDR3

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```

000059      30 CONTINUE
000060      IF(NDXMAC .EQ. 0) GO TO 35
000061      SUM=0.
000062      DO 31 N= 1, NDXMAC
000063      31 SUM= SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000064      AVMSLD = SUM/WTACMS
000065      35 CONTINUE
000066      IF((NDX1-NDXM) .EQ. 0) GO TO 40
000067      SUM=0.
000068      DO 32 N= N1,NDX1
000069      32 SUM = SUM+AVLD(N)*ABED(N)*DX*RHOSB(N)
000070      AVSGLD=SUM/WTSG
000071      40 CONTINUE
000072      DO 10 N=1,NDX
000073      10 WRITE (6,203)N, AVLD(N)
000074      1      , (W(NR,N),NR=1,NDR4)
000075      IF(TIME .LT. 1.1E-5) AVMSL1=AVMSLD
000076      IF(TIME .LT. 1.1E-5) AVSGL1=AVSGLD
000077      AVRCO2=WTACMS*(AVMSL1-AVMSLD)/TIME
000078      AVRH2O=WTSG*(AVSGL1-AVSGLD)/TIME
000079      DIMENSION F1(9),F2(9),F3(9),F4(9), F5(9),F6(9),F7(9),F8(9),F9(9)
000080      WRITE(6,205) F1,AVMSLD,F2,AVSGLD,F3,AVRCO2,F4,AVRH2O,F5,TOTKWH,
000081      F6,TOTHTC, F8,PCO2A, F9,VC02A
000082      205 FORMAT(////(9A6,F8.4,6X,9A6,F8.4 ))
000083      DATA F1/' AVG CO2 LOADING IN CO2 SORBENT (LB/LB)'/
000084      DATA F2/' AVG H2O LOADING IN DESICCANT (LB/LB)'/
000085      DATA F3/' TIME AVG CO2 DESORPTION RATE (LB/HR)'/
000086      DATA F4/' TIME AVG H2O DESORPTION RATE (LB/HR)'/
000087      DATA F5/' ELECTRICAL HEAT INPUT FROM START OF CYCLE (KWH)'/
000088      DATA F6/' HEAT ADDED BY COOLANT FROM START OF CYCLE (BTU)'/
000089      DATA F7/' CABIN CO2 PARTIAL PRESSURE (MM)'/
000090      DATA F8/' ACCUMULATOR CO2 PRESSURE (PSIA)'/
000091      DATA F9/' CO2 ACCUMULATOR VOLUME (CU FT)'/
000092
000093      C
000094      499 FORMAT(8H1BED NO. 13)
000095      100 FORMAT (1H0,16HDESORPTION CYCLE 13/
000096      1      3X,5HTIME=F9.5,1X2HHR,F12.3,1X,3HMIN,
000097      1      5X,15HTIME INCREMENT=F7.5,1X2HHR)
000098      101 FORMAT (//2X,10HAXIAL NODE,10X,14HTOTAL PRESS,MM,6X,14HGAS TEMP,DE
000099      1G F,5X,19HSORBENT TEMP, DEG F,2X,18HCOOLANT TEMP,DEG F,3X,19HMX CO
000100      2RE TEMP, DEG F )
000101      102 FORMAT(/(I9,11X,5(F14.4,6X)))
000102      103 FORMAT (/21HCO2 DESORPTION RATE=F7.4,1X5HLB/HR,5X,20HH2O DESORPTI
000103      10N RATE=F7.4,1X5HLB/HR)
000104      200 FORMAT (1H0/2X,10HAXIAL NODE,13X,9HMOLE FRAC,7X,
000105      12X,13HCO2 RATE,M/HR,6X,13HH2O RATE,M/HR)
000106      201 FORMAT(/(I9,11X,3(4X,F12.6,4X)))
000107      202 FORMAT (// 31HLOADING AT INTERIOR OF SORBENT//4X,4HSORB/4X,4HNOD
000108      1E,3X, 3HAvg, 9X,
000109      1      1H1,9X,1H2,9X,1H3,9X,1H4
000110      2      /6H AXIAL/5H NODE)
000111      203 FORMAT ( 15,4X,12(F6.4,4X))
000112      RETURN
      END

```



* ELT READ1,1,710712, 56801 , 1

```

000001      SUBROUTINE READ1
000002      COMMON/B1/
000003      1      ABED(20),AVC(20),ASC(20),ASX(20),AGX(20),AXC(20),
000004      2AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000005      3CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000006      4POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000007      5      NPSET(3),VDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORR(20)
000008      COMMON/B1A/
000009      1      HXG(20),HXS(20),HXC(20),HSG(20),
000010      2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,
000011      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000012      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
000013      NAMELIST/DB / ABED,AVC, ASX,AGX, AVX,RHOG,RHOSB,RHOS,RHOC,
000014      1RHOX,CPG, CPC,CPX,CPP,DX,NPSET,NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,
000015      2POUT,TIMET, PUMP,VPUMP,IDSORR,CPL,DP
000016      NAMELIST/DBA / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000017      1,WCC
000018      EQUIVALENCE(TCIN,T268)
000019      READ(5,DB)
000020      WRITE(6,DB)
000021      READ(5,DBA)
000022      WRITE(6,DBA)
000023      DO 10 N=1,NDX1
000024      10 ASG(N)=6.*RHOSB(N)/RHOS(N)/DP(N)
000025      RETURN
000026      END

```

* ELT READ2,1,710712, 56801 , 1

```

000001      SUBROUTINE READ2
000002      COMMON/B1D/
000003      1      HXG(20),HXS(20),HXC(20),HSG(20),
000004      2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,
000005      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000006      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
000007      NAMELIST/DBD / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000008      1,WCC
000009      EQUIVALENCE(TCIN,T268)
000010      READ(5,DBD)
000011      WRITE(6,DBD)
000012      RETURN
000013      END

```

* ELT READ3,1,710712, 56802 , 1

```

000001      SUBROUTINE READ3
000002      COMMON/B2/
000003      1      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000004      2AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000005      3CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000006      4POUT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000007      5      NPSET(3),VDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORR(20)
000008      COMMON/B2A/
000009      1      HXG(20),HXS(20),HXC(20),HSG(20),
000010      2SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,
000011      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000012      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VCO2A,SABCO2,TCO2A
000013      NAMELIST/MB / ABED,AVC, ASX,AGX, AVX,RHOG,RHOSB,RHOS,RHOC,
000014      1RHOX,CPG, CPC,CPX,CPP,DX,NPSET,NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,
000015      2POUT,TIMET, PUMP,VPUMP,IDSORR,CPL,DP
000016      NAMELIST/MBA / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000017      1,WCC
000018      EQUIVALENCE(TCIN,T268)
000019      DATA RHOG/ 20*0.0003/
000020      READ(5,MB)
000021      WRITE(6,MB)
000022      READ(5,MBA)
000023      WRITE(6,MBA)
000024      DO 10 N=1,NDX1
000025      10 ASG(N)=6.*RHOSB(N)/RHOS(N)/DP(N)
000026      RETURN
000027      END

```



* ELT READ4,1.710712, 56803 , 1

```
000001      SUBROUTINE READ4
000002      COMMON/B20/
000003      1          HXG(20),HXS(20),HXC(20),HSG(20),
000004      2SK(20),TKX(20),DH(20),DIF(20),GK(20),UC(20),T268,TOTCO2,TOTH20,
000005      3SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX
000006      1,TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VC02A,SABCO2,TC02A
000007      NAMELIST/MBD / HXG,HXS,HXC,HSG,SK,TKX,DH,DIF,GK, TCIN,HTR1,TMAX
000008      1,WCC
000009      EQUIVALENCE(TCIN,T268)
000010      READ(5,MBD)
000011      WRITE(6,MBD)
000012      RETURN
000013      END
```



* ELT START,1.710719, 62350 , 1

```

000001      SUBROUTINE START
000002      C
000003      COMMON/AD/ TG(20),PH2OI ,TGI ,PA ,      PK (2,20),PCO2I ,TS (20)
000004      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000005      2,TC2 (20),W (4,20),PT (20),      GMR ,GMW,GVIS, PN2,P02,
000006      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000007      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000008      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000009      6P0UT(10),TIMET(10),WTACMS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000010      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORR(20),
000011      8      HXG(20),HXS(20),HXC(20),HSG(20),
000012      9SK(20),TKX(20),OH(20),DIF(20),GK(20) ,UC(20),T268,TOTC02,TOTH20,
000013      1SUMPTM,AVMSL1,AVSGL1,HTR(20),TMAX,
000014      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VC02A,SABCO2, TC02A,
000015      1RS1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000016      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000017      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000018      3FR(2,20),      P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR2(20,4),CR3
000019      4(20,4), C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000020      5      WM(2),TIME,CYCLE,DT0,      DTMAX,WI,TI,PCO2C,
000021      6VOLCAB,RCO2C,
000022      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SARCOS
000023      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000024      1      CP1,CP2,X,      C1P,C2P,C3P,D1P
000025      C
000026      DO 5 N=1,NDX1
000027      I=IFN(N,NDXM)
000028      CPS(N)=CPP(N)+W(1,N)*CPL(I)
000029      5 RS(N)=DP(N)/2.000
000030      DO 30 N= 1, NDX1
000031      30 VOIDF(N) = 1. - RHOSB(N)/RHOS(N)
000032      DO 115 N=1,NDX1
000033      115 A(N)= GMR/ABED(N)/PA/GMW
000034      NDR=NDR4-1.
000035      NDR2= 2*NDR
000036      NDR3=NDR2+1
000037      DO 10 I=1,NDX1
000038      VS(I)=4./3.*3.1416*RS(I)**3
000039      DVS(I)=VS(I)/NDR
000040      DVS1(I)=DVS(I)/2
000041      RS1(I,1)=0.
000042      DO 10 K=2,NDR3
000043      10 RS1(I,K)=CBRT(3./4./3.1416*(4./3.*3.1416*RS1(I,K=1)**3+DVS1(I)))
000044      DO 11 I=1,NDX1
000045      CR1(I,1)=DVS1(I)*RHOS(I)
000046      CR2(I,1)=0.
000047      CR3(I,1)=4.*3.1416*RS1(I,2)**2*DIF(I)/(RS1(I,3)-RS1(I,1))*RHOS(I)
000048      DO 11 K=2,NDR4
000049      CR1(I,K)=DVS(I)*RHOS(I)
000050      CR2(I,K)=4.*3.1416*RS1(I,2*K-2)**2*DIF(I)/(RS1(I,2*K-1)-RS1(I,2*K-
000051      13))*RHOS(I)
000052      11 CR3(I,K)=4.*3.1416*RS1(I,2*K)**2*DIF(I)/(RS1(I,2*K+1)-RS1(I,2*K-1)
000053      1)*RHOS(I)
000054      DO 12 N=1,NDX1
000055      12 CR1(N,NDR4)=CR1(N,1)
000056      RETURN
000057      END

```



• ELT TGLCOL,1,710514, 58260 , 1

```

000001      SUBROUTINE TGLCOL(TC,NDXMAX,UC,RHOC,CPC,CX,AXC,HXC,T268,DX,DT,
000002      1AVC,NOGLIN,DT0,T81,TS2,TX1,TX2,TC1,TC2)
000003      DIMENSION C1(20),C2(20),C3(20),D(20),TC(1),TX(1),HXC(1),AVC(1),
000004      1      TS1(1),T82(1),TX1(1),TX2(1),TC1(1),TC2(1)
000005      DIMENSION UC(1),RHOC(1),CPC(1),AXC(1)
000006      DN=DT+DT0
000007      DO 10 N=1,NDXMAX
000008      CC1=-UC(N)
000009      CC2=HXC(N)/(CPC(N)*RHOC(N))*AVC(N)*0.5
000010      IF( UC(N) .GT. 0.) GO TO 5
000011      C3(N)=-CC1/DX
000012      C2(N)=1./DN+CC2-C3(N)
000013      C1(N)=0.0
000014      GO TO 10
000015      5 C1(N) = CC1/DX
000016      C2(N) = 1./DN + CC2 - C1(N)
000017      C3(N) = 0.0
000018      10 D(N)=TC2(N)/DN+CC2*TX1(N)*2. - CC2*TC2(N)
000019      C1(NOGLIN) = 0.
000020      C3(NOGLIN) = 0.
000021      D(NOGLIN)=D(NOGLIN) +ABS(UC(NOGLIN))/DX*T268
000022      CALL FDEGIM(C1,C2,C3,D,TC,NDXMAX)
000023      RETURN
000024      END
    
```

• ELT TSORB,1,710719, 62351 , 1

```

000001      SUBROUTINE TSORB
000002      COMMON/AD/ TG(20),PH201 ,TGI ,PA ,      PK (2,20),PCO2I ,TS (20)
000003      1;TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),
000004      2TC2 (20),W (4,20),PT (20),      GMR ,GMW,GV16, PN2,PO2,
000005      3      ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),
000006      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),
000008      6POUT(10),TIMET(10),WTACHS,WTSG ,PUMP(10),VPUMP(10),CPP(20),
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),
000010      8      HXG(20),HXS(20),HXC(20),HSG(20),
000011      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,
000012      1SUMPTH,AVMSL1,AVSGL1,HTR(20),TMAX,
000013      1TOTKWH,HTR1(20),WC,TOTHTC,WCC,PCO2A,VC02A,SABCO2, TCO2A,
000014      1RB1(20,9),      A(20),F(20),C(20),VS(20),DVS(20),DVS1(20),RS(20),
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),
000017      3FR(2,20),      P1(20),P2(20),P3(20),WB(20),CR1(20,4),CR2(20,4),CR3
000018      4(20,4),      C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),
000019      5      WM(2),TIME,CYCLE,DT0,      DTMAX,WI,T1,PCO2C,
000020      6VOLCAB,RCO2C,
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,
000023      1      CP1,CP2,X,      C1P,C2P,C3P,D1P
000024      DIMENSION S1(41),S2(41),S3(41),B1(41)
000025      DO 10 N=1,NDX1
000026      T=(DT+DT0)/CPS(N)/RHOSB(N)
000027      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))
000028      C61(N)=CS1(N)*(1.0+T1)
000029      C62(N)=CS2(N)*(1.0+T1)
000030      B1(N) =TS2(N)*CS1(N)*PT(N)-CS2(N)*(P1(N)+P2(N))*(W(NDR4,N)-WS(N))+
000031      1P3(N)*PT(N))+T*(ASG(N)*HSG(N)*TC (N)+ASX(N)*HXS(N)*
000032      2      TX1(N))-T1*T82(N)
000033      S1(N)=-T*SK(N)/DX/DX
000034      S2(N)=1.-2.*S1(N)+T1
000035      S3(N)=S1(N)
000036      10 CONTINUE
000037      S2(1)=S2(1)+S1(1)
000038      S1(1)=0.0
000039      S2(NDX1)=S2(NDX1)+S3(NDX1)
000040      S3(NDX1)=0.
000041      NSG=NDXM+1
000042      S2(NDXM)=S2(NDXM)+S3(NDXM)
000043      S3(NDXM)=0.
000044      S2(NSG) = S2(NSG)+S1(NSG)
000045      S1(NSG)=0.0
000046      CALL FDEGIM(S1,S2,S3,B1,TS,NDX1)
000047      RETURN
000048      END
    
```


ELT TSORBA,1,710719, 62352 , 1

```

000001      SUBROUTINE TSORBA
000002      COMMON/AD/ TG(20),PH201 ,TGI ,PA ,          PK (2,20),PC021 ,TS (20)      *NEW
000003      1,TC (20),TX (20), TS1 (20),TS2 (20),TX1 (20),TX2 (20),TC1 (20),      *NEW
000004      2TC2 (20),W (4,20),PT (20),          GMR ,GMW,GVIS, PN2,P02,      *NEW
000005      3          ABED(20),AVC(20),ASG(20),ASX(20),AGX(20),AXC(20),      *NEW
000006      4AVX(20),RHOG(20),RHOSB(20),RHOS(20),RHOC(20),RHOX(20),      *NEW
000007      5CPG(20),CPC(20),CPX(20),CPS(20),DX,CPL(2),DP(20),      *NEW
000008      6POUT(10),TIMET(10),WTACHS,WTSG ,PUMP(10),VPUMP(10),CPP(20),      *NEW
000009      7NPSET(3),NDR4,NDXMAC,NBCOUT,NDX1,NDXM,NOG,IDSORB(20),      *NEW
000010      8          HXG(20),HXS(20),HXC(20),HSG(20),      *NEW
000011      9SK(20),TKX(20),DH(20),DIF(20),GK(20) ,UC(20),T268,TOTCO2,TOTH20,      *NEW
000012      1SUMPTN,AVMSL1,AVSGL1,HTR(20),TMAX,      *NEW
000013      1 TOTKWH,HTR1(20),WC,TOTHTC,WCC,PC02A,VCO2A,SABC02, TC02A,      *NEW
000014      1RS1(20,9),          A(20),F(20),C(20),VS(20),DVS1(20),RS(20),      *NEW
000015      1UG(20),PS(20),DS(20),CS1(20),CS2(20),C1(4,20),C2(4,20),D1(4,20),      *NEW
000016      2D2(20),PC1(20),PC2(20),PC3(20),C1P(20),C2P(20),C3P(20),D1P(20),      *NEW
000017      3FR(2,20),          P1(20),P2(20),P3(20),WS(20),CR1(20,4),CR3      *NEW
000018      4(20,4),          C3(4,20),B(4,20),Q(4,20),CP1(20),CP2(20),X(20),VOIDF(20),      *NEW
000019      5          WM(2),TIME,CYCLE,DT0,          DTMAX,WI,TI,PC02C,      *NEW
000020      6VOLCAR,RC02C,      *NEW
000021      7NCYCLT,NPRINT,NCYCLE,NDTCON,NTEMP,NSTART,NPR,DT,DTT(4),SABCOS      *NEW
000022      DOUBLE PRECISION C1,C2,D1,D2,PC1,PC2,PC3,P1,P2,P3,C3,Q,B,      *NEW
000023      1          CP1,CP2,X,          C1P,C2P,C3P,D1P      *NEW
000024      DIMENSION S1(41),S2(41),S3(41),B1(41)      *NEW
000025      DO 10 N=1,NDX1      *NEW
000026      T=(DT+DT0)/CPS(N)/RHOSB(N)      *NEW
000027      T1=0.5*T*(ASG(N)*HSG(N)+ASX(N)*HXS(N))      *NEW
000028      CS1(N)=CS1(N)*(1.0+T1)      *NEW
000029      CS2(N)=CS2(N)*(1.0+T1)      *NEW
000030      J=JFN(N,NDXM)      *NEW
000031      TGAVG1=TG(N)      *NEW
000032      B1(N) =TS2(N)*CS1(N)*      *NEW
000033      1PK(I,N),      *NEW
000034      2          -CS2(N)*(P1(N)+P2(N)*(W(NDR4,N)-WS(N))+      *NEW
000035      1P3(N)*      *NEW
000036      2PK(I,N)      *NEW
000037      3          )+T*(ASG(N)*HSG(N)+TGAVG1+      *NEW
000038      4ASX(N)*HXS(N)+TX1(N))-T1*TS2(N)      *NEW
000039      S1(N)=-T*SK(N)/DX/DX      *NEW
000040      S2(N)=1.-2.*S1(N)+T1      *NEW
000041      S3(N)=S1(N)      *NEW
000042      10 CONTINUE      *NEW
000043      S2(1)=S2(1)+S1(1)      *NEW
000044      S1(1)=0.0      *NEW
000045      S2(NDX1)=S2(NDX1)+S3(NDX1)      *NEW
000046      S3(NDX1)=0.      *NEW
000047      NSG=NDXM+1      *NEW
000048      S2(NDXM)=S2(NDXM)+S3(NDXM)      *NEW
000049      S3(NDXM)=0.      *NEW
000050      S2(NSG)= S2(NSG)+S1(NSG)      *NEW
000051      S1(NSG)=0.0      *NEW
000052      CALL FDEQIM(S1,S2,S3,B1,TS,NDX1)      *NEW
000053      RETURN      *NEW
000054      END      *NEW

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@ ELT XYZMAP,1,710514, 38520 , 1

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000001      FUNCTION XYZMAP(IND,X,Y,NP,Z,NC,IDX,IDY,BX,BY,ANS)
000002      C
000003      C      FUNCTION XYZMAP HAS THE CAPABILITY OF SUBROUTINES MAPRDY + LAGIN2.
000004      C      ANSWER IS ALSO AVAILABLE AT LOCATION (ANS).
000005      C      ALSO CAPABLE OF HANDLING MAP THAT HAS Z-LINES CROSSING EACH OTHER.
000006      C
000007      C      X=ABSISSA, Y=ORDINATE, Z=THIRD PARAMETER.
000008      C
000009      C      IND=0, Z=F(X,Y), (EQUIVALENT TO SUBROUTINE MAPRDY).
000010      C      IND=1, Y=F(X,Z), (EQUIVALENT TO SUBROUTINE MAPRDY).
000011      C      IND=-1, Y=F(X) ONLY, (EQUIVALENT TO LAGIN2), THEN Z,NC,IDY, AND AY
000012      C      ARE DUMMY VARIABLES THAT ARE NOT NEEDED IN ACTUAL INTERPOLATION.
000013      C
000014      C      XS MUST BE STORED IN ASCENDING ORDER FOR EACH Z, SIMILARLY,
000015      C      SMALLEST Z BE FED IN AS Z(1), ZS ARE IN ASCENDING ORDER.
000016      C      XS NEED NOT BE THE SAME VALUES FOR VARIOUS ZS.
000017      C      X,Y AND Z ARE TO BE DIMENSIONED IN THE MAIN (OR CALLING) PROGRAM,
000018      C      THEY MUST BE DIMENSIONED NOT LESS THAN *** X(NP*NC), Y(NP*NC) AND
000019      C      Z(NC) *** NOTE NC MAY NOT BE GREATER THAN 20 ***
000020      C
000021      C      NP=NUMBER OF POINTS PER CURVE (OR NUMBER OF X,Y PAIRS FOR EACH Z).
000022      C      NC=NUMBER OF CURVES (OR NUMBER OF ZS), 1 TO A MAXIMUM OF 20
000023      C
000024      C      IDX=POINTS USED FOR INTERPOLATION IN X-DIRECTION,
000025      C      IDY=POINTS USED FOR INTERPOLATION IN Y-DIRECTION (IND=0),
000026      C      OR IN Z-DIRECTION (IND=1).
000027      C      IDX OR IDY CAN EITHER BE 2 OR 3 ONLY.
000028      C      BX=FIRST INDEPENDENT VARIABLE.
000029      C      BY=SECOND INDEPENDENT VARIABLE, (WHEN IND=0 OR 1 ONLY).
000030      C      BY=Y INDEPENDENT VARIABLE, WHEN (IND=0).
000031      C      BY=Z INDEPENDENT VARIABLE, WHEN (IND=1).
000032      C      ANS=DEPENDENT VARIABLE Z(X=AX,Y=AY), WHEN IND=0.
000033      C      ANS=DEPENDENT VARIABLE Y(X=AX,Z=AY), WHEN IND=1.
000034      C      ANS=DEPENDENT VARIABLE Y(X=AX), WHEN IND=-1.
000035      C
000036      C      NO PRINT OUT, IF DATA OFF THE RANGE OF MAP OR CURVE.
000037      C      THEN, USE 2-POINT INTERPOLATIONS AUTOMATICALLY.
000038      C
000039      C
000040      C      *****
000041      C      XS, YS, AND ZS ARE READ IN IN MAIN PROGRAM RECOMMENDED AS FOLLOWS,
000042      C4100 FORMAT(8I10) *****
000043      C4101 FORMAT(8F10.0) *****
000044      C      ***** FOR IND=0 OR 1 *****
000045      C4101 READ (5,4100) NP,NC *****
000046      C      DO 100 N=1,NC *****
000047      C      READ (5,4101) Z(N) *****
000048      C      ME=N*NP *****
000049      C      MS=ME-NP+1 *****
000050      C 100 READ (5,4101) (X(M),Y(M),M=MS,ME) *****
000051      C      ***** FOR IND=-1 *****
000052      C      READ (5,4100) NP *****
000053      C      READ (5,4101) (X(M),Y(M),M=1,NP) *****
000054      C      *****
000055      C      DIMENSION X(2),Y(2),Z(2),ZZ(20),ZX(20)
000056      C      JS=1
000057      C      IF (IND) 105,106,103
000058      C 103 DO 104 I=1,NC

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000059      104 ZX(I)=Z(I)
000060          GO TO 141
000061      105 JE=1
000062          GO TO 108
000063      106 DO 107 I=1,NC
000064      107 ZZ(I)=Z(I)
000065          JE=NC
000066          NCROSS=0
000067      108 DO 126 J=JS,JE
000068          JX2=(J-1)*NP
000069          DO 109 I=1,NP
000070          J2=I+JX2
000071          IF (BX-X(J2)) 114,110,109
000072      109 CONTINUE
000073          GO TO 119
000074      110 ANS=Y(J2)
000075          GO TO 123
000076      114 IF(1-IDX)120,120,119
000077      119 JX2=J2-IDX
000078      120 IS=JX2+1
000079          IE=JX2+IDX
000080          IF(IDX.GT.2) GO TO 122
000081      121 ANS=(Y(IE)*(BX-X(IS))-Y(IS)*(BX-X(IE)))/(X(IE)-X(IS))
000082          GO TO 123
000083      122 IM=IS+1
000084          G1=(BX-X(IS))/(X(IM)-X(IE))
000085          G2=(BX-X(IM))/(X(IE)-X(IS))
000086          G3=(BX-X(IE))/(X(IS)-X(IM))
000087          ANS=-Y(IS)*G2*G3-G1*(Y(IM)*G3+Y(IE)*G2)
000088      123 IF (IND) 158,125,124
000089      124 ZZ(J)=ANS
000090          GO TO 126
000091      125 ZX(J)=ANS
000092          IF(ANS.LT.ZX(1)) NCROSS=1
000093      126 CONTINUE
000094          IF(IND.NE.0) GO TO 151
000095          IF(NCROSS.EQ.0) GO TO 141
000096      C
000097          DO 130 K=2,NC
000098          JMIN=K-1
000099          DO 129 IP=K,NC
000100          IF (ZX(IP)-ZX(JMIN)) 128,128,129
000101      128 JMIN=IP
000102      129 CONTINUE
000103          IK=K-1
000104          C1=ZX(JMIN)
000105          Z1=ZZ(JMIN)
000106          ZX(JMIN)=ZX(IK)
000107          ZZ(JMIN)=ZZ(IK)
000108          ZX(IK)=C1
000109      130 ZZ(IK)=Z1
000110      C
000111      141 ICPY= IDY-1
000112          DO 142 I=1,NC
000113          IF(BY-ZX(I))145,144,142
000114      142 CONTINUE
000115          JS=NC-ICPY
000116          GO TO 147
000117      144 JS=I
000118          IF (IND.EQ.0) GO TO 151

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000119          JE=JS
000120          GO TO 108
000121          145 IF(I.LE.IDY) GO TO 147
000122          146 JS=I-ICPY
000123          147 JE=JS+ICPY
000124          IF (IND) 108,1152,108
000125          C   Y=F(X,Z) OR Z=F(X,Y) CALCULATION DEPENDING ON IND=0 OR 1.
000126          151 ANS=ZZ(JS)
000127          GO TO 158
000128          1151 IF(JE.EQ.JS) GO TO 151
000129          1152 IF(IDY.GT.2) GO TO 153
000130          152 ANS=(ZZ(JE)*(BY-ZX(JS))-ZZ(JS)*(BY-ZX(JE)))/(ZX(JE)-ZX(JS))
000131          GO TO 158
000132          153 JM=JS+1
000133          G1=(BY-ZX(JS))/(ZX(JM)-ZX(JE))
000134          G2=(BY-ZX(JM))/(ZX(JE)-ZX(JS))
000135          G3=(BY-ZX(JE))/(ZX(JS)-ZX(JM))
000136          ANS=-ZZ(JS)*G2*G3+G1*(ZZ(JM)*G3+ZZ(JE)*G2)
000137          158 XYZMAP=ANS
000138          RETURN
000139          END

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