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USER'S MANUAL FOR SOLID PROPULSION OPTIMIZATION CODE (SPOC)

Volume III - Program Description

Author: G. P. Roys

Thiokol Corporation
Huntsville Division
Huntsville, AL 35807

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Prepared for

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AIR FORCE SYSTEMS COMMAND
EDWARDS AFB, CALIFORNIA 93523

NOTICES

FOREWORD

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JOHN H. COSTELLO, JR, 1Lt, USAF
Project Manager

LEE G. MEYER, Chief
Air-Launched Missile
Propulsion Branch

FOR THE COMMANDER

CHARLES R. COOKE
Director, Solid Rocket Division

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number): Solid propellant rocket motor, mathematical modeling, numerical non-linear optimization, computer code, preliminary design
20. ABSTRACT (Continue on reverse side if necessary and identify by block number):

This report is Volume III of a three-volume user's manual for a computer code that performs detailed preliminary designs of solid propellant rocket motors. All major components and performance of a motor are mathematically determined using source dimensions and characteristics. A direct pattern search nonlinear optimization scheme based on the Hooke and Jeeves algorithm is employed to establish motor characteristics that optimize any one of several performance parameters. Decision variables during optimization

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20. are propellant formulation, propellant burn rate, propellant grain dimensions, nozzle dimensions, and pressure vessel dimensions. Provisions are made for easily inserted user-defined models of several characteristics. Constraints imposed during the optimization process are performance requirements, design constraints, and operating limits.

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VOLUME III

PROGRAM DESCRIPTION

INTRODUCTION

The Solid Propulsion Optimization Code (SPOC) performs detailed preliminary designs of a large variety of solid propellant rocket motors. Dimensions of the propellant grain, nozzle, and pressure vessel are adjusted by the code, along with propellant formulation and burn rate, to produce a motor design that satisfies performance requirements and design constraints, and that has been optimized with respect to a user-selected parameter.

This volume of the User's Manual - Volume III (Program Description) - contains the subroutine descriptions and flow charts, and cross-indices of common statements, subroutines and call statements. Volume I (Technical Description) gives the basis for the code computations analytical development, logic flow charts used in verification checks and error messages. Volume II (User's Guide) contains the input and output dictionaries and their accompanying illustrations, along with other input instructions needed to execute the code.

SUBROUTINE DESCRIPTIONS

ABMODL	Calculates combustion response per analytical response model. Used by subroutine RSPNSE.
ACCEL	Calculates missile horizontal and vertical acceleration. A point-mass missile is assumed to be flying a ballistic trajectory in the altitude-range plane.
ACOUST	Calculates velocity of acoustic volume current at end of motor. Used by subroutine MODCLC.
AF2SUB	Solves for port perimeter and area of Type 2 configurations for each plane. This is a 2-dimensional solution and is called by LP2SUB. See Note 1.
ARC	Surface area computational subroutine used with forward propellant segment of conocyl grain.
AREAS	Surface area computational subroutine used with forward propellant segment of conocyl grain. Calls LOOK1 and LOOK2, which are separate entries in subroutine ELIPS.
ASESUB	Calculates surface areas and volumes of individual segments and end sections by calling RASUB, XRSUB, LRSUB and HESUB. These break the configuration down into equivalent dimensions for a simplified configuration.
AS2SUB	First level geometry for end closures of type 2 configurations. This is a 3-dimensional calculation. Being primarily an executive routine, it calls ASESUB, AWESUB and RCSUB. See Note 1.
AS3SUB	First level geometry for end closures of type 3 configurations. This is a 3-dimensional calculation. Being primarily an executive routine, it calls ASESUB, AWESUB, HESUB, and RCSUB. See Note 1.
ATAESB	Calculates nozzle throat area (AT) and exit area (AE at any time during ballistic simulation.
ATMOS	Calculates atmospheric properties as a function of altitude for (1) 1959 ARDC STD DAY; (2) MIL-STD-210A TROPICAL DAY; (3) MIL-STD-210A POLAR DAY; (4) MIL-STD-210A HOT DAY; (5) MIL-STD-210A COLD DAY.
AWESUB	Calculates areas and volumes for the web segment of a type 2 configuration. A 3-dimensional end routine. See Note 1.

Subroutines in SPOC (Continued)

BLDATA	Block data for thermochemistry: Atomic Symbols, Atomic Weights, Valences.
CASEAN	Calculates case wall thickness, forward and aft closure thicknesses and weight summary of case structural parts. Calls WACL1, WFCL1, and WF2A3, which are separate entries in subroutine CLOS.
CFVLSB	Calculates $C_{F_{v\lambda}}$ (thrust coefficient for vacuum conditions corrected for divergence losses). λ_n is brought into this subroutine.
CHEKIN	An input checking and diagnosis routine. Prints messages that describes the problem the user has set up.
CLOS	Case forward and aft closure computational routine. Calculates geometric details for three forward closure types and two aft closure types, plus associated volumes and weights.
COMP	Executive (Main Logic Control) routine. Calls all other analysis modules.
CPHS	Calculation of thermodynamic properties of individual species. Part of thermochemistry module.
CROSS1	Sets up for subroutine ACOUST. Used by subroutine MODCLC.
CROSS2	Detects sign change (zero) of acoustic volume current velocity to within convergence tolerances. Used by subroutine MODCLC.
DPRINT	D-array summary print routine. The D-array is the list of variables upon which the optimizer is allowed to operate.
ECSUB	Calculates and tests constants that deal with the end closure; primarily tests.
ELIPS	Grain regression computational routine for conocyl grain with elliptical forward closure.
EQLBRM	Calculates equilibrium composition and properties of propellant combustion species. Part of thermochemistry module.
EXIT	Universal exit to give print-out of current values of PATSH-adjusted parameters when there is an abnormal termination of code execution.

Subroutines in SPOC (Continued)

E488M2	Executive subroutine for stability analyses. Calls all other subroutines. Calculates and writes stability penalty.
FIG5	Table look-up for photoelastic stress parameter HSTAR versus valley included angle to use with star grain configuration.
FIG6	Table look-up for photoelastic stress parameter HSTAR versus valley width to use with star grain configuration.
FIG7	Table look-up for photoelastic stress parameter HSTAR versus valley included angle to use with wagon-wheel grain configuration.
FLT	Calculates ideal drag-free velocity at end of motor operation and maximum axial acceleration during motor operation.
FPACC	Part of missile flight dynamics logic. A diagnostic routine used in the computation of missile acceleration along the flight path.
GAUSS	Solution of N simultaneous linear equations. Used in thermochemistry module.
G2F2FG	Calculates functions used in calculation of stability integrals. Used by subroutine INTGL.
HESUB	Calculates the distance from the last cylindrical portion plane to the end of the end section for given distances from motor centerline.
HITEMP	Computes motor operating limit parameters with high temperature grain and compares them to requirements.
IBSUB	Internal Ballistics Subroutine - Calculates all gas flow properties between any two adjacent planes. This is the heart of subroutine SEC3SB.
IMPEFF	Computes rocket motor impulse efficiency using SPP empiricisms (Ref. AFRPL-TR-75-36).
INPUT	Reads namelist STABIN. Sorts incoming data set from common/TIMDAT/. Calculates pressure and velocity exponents. Prints input data.
INTGL	Calculates stability integrals. Used by subroutine E488M2.
ITERP1	Nth order interpolation of a table having a single independent variable.

Subroutines in SPOC (Continued)

LIQUID	Part of thermochemistry input diagnostics. Checks numerical compatibility of amounts of liquid ingredients input and total solids level.
LOTEMP	Computes motor operating limit parameters with low temperature grain and compares them to requirements.
LP1SUB	Calculates the port perimeter and area for type 1 configurations at each plane. See Note 1.
LP2SUB	Calculates the port perimeter and area for type 2 configurations at each plane. See Note 1.
LP3SUB	Calculates the port perimeter and area for type 3 configurations at each plane. See Note 1.
LP4SUB	Calculates the port perimeter and area for type 4 configurations at each plane. See Note 1.
LRSUB	Calculates the section of the perimeter between radii in the end section.
MACHNO	Solution for mach number from area ratio and specific heat ratio. Ideal, one-dimensional, single phase gas dynamics are assumed.
MAINCO	Executive (main control) routine for thermochemistry computation once the incoming ingredient weight fraction set has been checked for numerical validity and for compatibility with user-input limits.
MATRIX	Matric solution used in thermochemistry module.
MODCLC	Detects acoustic mode frequency by convergence on zeros of acoustic volume current velocity. Used by E488M2.
MTRCST	Calculates development, qualification, PFRT and production costs for steel case motors using Tri-Services cost model.
NEWING	Manipulative routine for modification of thermochemistry logic by adding new ingredients
NEWRAP	Newton-Raphson iterative solution of an implicit function.

Subroutines in SPOC (Continued)

NORMAL	Adjusts incoming set of propellant ingredient weight fractions so that total equals 1.0. Adjusts only those ingredients that user has specified for adjustment during optimization process.
NOZINP	Nozzle configuration data reading, check, and print. Determines geometric validity of incoming data set.
NOZL	Calculates nozzle geometry from incoming data set. Performs thermal and structural analyses. Calculates weight.
NOZZSB	Lists nozzle parameters used by ballistic simulation module and checks them. It is called by subroutine SEC1SB.
NREQ1	Iterative solution for a dimension (ALPHMX) of Type 1 (Star) grain required by ballistic simulation module.
NREQ2	Iterative solution for a dimension (AFSTAR) of Type 1 (Star) grain required by ballistic simulation module.
NREQ3	Iterative solution for a dimension (AFSTAR) of Type 1 (Star) grain required by ballistic simulation module.
NREQ4	Iterative solution for a dimension (BETAX) of Type 1 (Star) grain required by ballistic simulation module.
NREQ5	Iterative solution for a dimension (DELTA) of Type 1 (Star) grain required by ballistic simulation module.
NREQ6	Iterative solution for a dimension (GAMMA) of Type 1 (Star) grain required by ballistic simulation module.
NREQ7	Iterative solution for a dimension (GAMMA) of Type 2 (Wagon Wheel) grain required by ballistic simulation module.
NREQ8	Iterative solution for a dimension (GAMMA) of Type 2 (Wagon Wheel) grain required by ballistic simulation module.
NREQ9	Iterative solution for a dimension (GAMMA) of Type 2 (Wagon Wheel) grain required by ballistic simulation module.

Subroutines in SPOC (Continued)

ONETMP	Calculates operating limits and associated penalties when ballistic simulation is performed at only one grain temperature.
OUT1	Converts part of thermochemical calculation results to proper units and rocket definitions. Called by RKTOUT.
PATSH	Pattern search optimization routine.
PCGSUB	Is a general solution of plane constants for either side of a Type 2 configuration. It does the calculations for PC2SUB. See Note 1.
PC1SUB	Prints input table of "Thickness, Perimeter and Port Area"; checks geometry values and completes geometry print-out; calls LP1SUB; and prints "Initial Perimeter, Initial Port Area and Inert Sliver" values for Type 1 configurations. All of this is seen in geometry part of the print-out. See Note 1.
PC2SUB	Prints out the geometry section of the input data for Type 2 configurations. This routine is primarily executive. It calls LP2SUB and PCGSUB. See Note 1.
PC3SUB	Prints out the geometry section of the input data for Type 3 configurations. See Note 1.
PC4SUB	Prints out geometry input data; calls LP4SUB and prints out "Initial Perimter, Initial Port Area and Inert Sliver" data for Type 4 configurations. See Note 1.
PEPCSB	Calculates ratio of pressure at the nozzle exit to pressure in the chamber. This is an iterative solution.
PROPST	Performs grain structural analysis.
PTLSTB	Calculates stability margin (linear alpha) and damping coefficient. Prints stability summary and details. Used by subroutine E488M2.
RASUB	Calculates the radius to any point on the burning surface perimeter in the end sections.

Subroutines in SPOC (continued)

RATESB	Calculates burn rate as a function of pressure and Mach number. Called mainly by subroutine IBSUB.
RCSUB	Calculates radius from the motor centerline to the closure in the end sections.
REACT	Locates propellant ingredients in internal tables in thermochemistry module and sets proper indices for locating elements and coefficients.
RKTOUT	Converts part of thermochemical calculation results to proper units and rocket definitions. Calls OUT3, a second entry to subroutine OUT1.
ROCKET	Converts part of thermochemical calculation results to proper units and rocket definitions. Calls NEWOF, a second entry to subroutine SAVE.
RSPNSE	Calculates combustion response per selected response option (four different models) for each section of the motor. Used by subroutine E488M2.
RTCKSB	Checks for validity of the burn rate inputs.
SAVE	Saves thermochemical data for subsequent passes with same ingredients to speed solution.
SBPHAT	Calculates the acoustic pressure at a specific location in the motor. Used by subroutine STBINT.
SBQBAR	Calculates the mean flow volume current at a specific location in the motor. Used by subroutine STBINT.
SEARCH	Looks for thermodynamic coefficients of combustion species using indices created by subroutine REACT.
SEC1SB	Determines the number of input planes. Interpolates between plane inputs. Computes plane constants by calling PC(1,2,3 or 4) SUB depending on the type geometry. Computes head end and nozzle end constants by calling ECSUB. Computes initial volumes. Checks scale factor inputs and sets SF = 1.0 if scale factors are not used. Checks nozzle diameter inputs by calling NOZZSB. Checks time increment inputs. Checks burning rate inputs by calling RTCKSB. Prints all the values it calculated or checked.

SEC2SB	Computes end section surface areas and volumes by calling LP(2 or 3)SUB and AS(2 or 3)SUB depending on the geometry. Computes perimeters and port areas by calling LP(1,2,3 or 4)SUB depending on the geometry. Calculates fuel areas, incremental surface areas, and propellant volumes. Computes interpolations on burn rate scale factors if they are used. Computes nozzle throat and exit areas by calling ATAESB. Computes ballistic performance by calling SEC3SB. Updates time and web thickness for next increment. Goes back to the first of the subroutine for the next-time calculations.
SEC3SB	Calculates ballistic constants. Computes ballistics for the head-end and nozzle-end segments by calling RATESB and IBSUB in sets. Computes nozzle section ballistics as in the head end. Checks mass generated with mass discharged for equilibrium. Adjusts pressure for new run if equilibrium is not reached. Computes thrust and integrals. Resets initial conditions for the next time increment. Statement 50 is the beginning of the main ballistic loop.
SETUP1	Input validity tests and geometry setup for communication with ballistic simulation module for grain Type 1 (Star). See Note 2.
SETUP2	Input validity tests and geometry setup for communication with ballistic simulation module for grain Type 2 (Wagon Wheel). See Note 2.
SETUP3	Input validity tests and geometry setup for communication with ballistic simulation module for grain Type 3 (Finocyl). See Note 2.
SETUP4	Input validity tests and geometry setup for communication with ballistic simulation module for grain Type 4 (Conocyl). See Note 2.
SETUP5	Input validity tests and geometry setup for communication with ballistic simulation module for grain Type 5 (CP). See Note 2.
STBDAT	Creates matrix of grain dimensions and internal gas dynamic conditions for use by combustion stability module. Called by SEC3SB. Calls STBCLO and STBNOZ (which are separate entries into CLOS and NOZL, respectively).

Subroutines in SPOC (Contined)

STBINT	Calculates the stability integrals for each section of the motor. Used by subroutine E488M2.
TCHEM	Executive subroutine for propellant thermochemical analysis module. Called by subroutine COMP.
TRAJ	Trajectory flight dynamics computational routine. Point mass missile flying two dimensional ballistic trajectory in altitude range plane. Fourth order Runge-Kutta numerical integration.
TRAJIN	Trajectory data read, decision logic, and print routine.
UBCALC	Calculates constants describing geometry (perimeter and port area) and mean flow volume current for each section of the motor. Used by subroutine E488M2.
USERCS	User-supplied cost model.
USEREF	User-supplied impulse efficiency model.
USERRB	User-supplied propellant burn rate model.
USERRH	User-supplied propellant rheological properties model.
USERSE	User-supplied propellant strain endurance model.
VOLUME	Component volume computational routine for nozzle analysis subroutine NOZL.
XRSUB	This routine calculates the distance (XR) from the boundary of a symmetrical segment to the perimeter. This is used by the end section subroutines.

NOTES

1. Grain type numbers in noted definitions are designations internal to the ballistic simulation module and are not the same as the grain types available in SPOC.

2. Calls AFTCL1, AFTCL2, FCL2A3, and FWDCL1, which are separate entries in subroutine CLOS.

SUBROUTINE CROSS-INDEX

Subroutine		Called by These Subroutines					
ABMODL		RSPNSE					
ACCEL		TRAJ					
ACOUST		MODCLC					
AFTCL1	E	CLOS	SETUP1	SETUP2	SETUP3	SETUP4	SETUP5
AFTCL2	E	CLOS	SETUP1	SETUP2	SETUP3	SETUP4	SETUP5
AF2SUB		LP2SUB					
ARC		AREAS					
AREAS		SETUP4					
ASESUB		AS2SUB	AS3SUB				
AS2SUB		SEC1SB	SEC2SB				
AS3SUB		SEC1SB	SEC2SB				
ATAESB		SEC2SB					
ATMOS		ACCEL	TRAJIN				
AWESUB		AS2SUB	AS3SUB				
BLDATA							
CASEAN		COMP					
CFVLSB		SEC3SB					
CHECKIN		MAIN					
CLOS		SETUP1	SETUP2	SETUP3	SETUP4	SETUP5	
COMP		MAIN					
CPHS		EQLBRM					
CROSS1		MODCLC					
CROSS2		MODCLC					
DPRINT		COMP					
ECSUB		SEC1SB					
ELIPS		AREAS					
EQLBRM		ROCKET					
EXIT		AWESUB	CNTRL	COMP	ELIPS	E488M2	FPACC
		INPUT	MODCLC	NOZINP	SEC3SB	SETUP1	SETUP2
		SETUP3	SETUP4	SETUP5	TCHEM	TRAJIN	
E488M2		COMP					
FCL2A3	E	CLOS	SETUP1	SETUP2	SETUP3	SETUP5	
FIG5		PROPST					
FIG6		PROPST					
FIG7		PROPST					
FLT		COMP					
FPACC		TRAJ					
FWDCL1	E	CLOS	SETUP1	SETUP2	SETUP3	SETUP4	SETUP5
GAUSS		EQLBRM					
G2F2FG		INTGL					
HESUB		ASESUB	AS3SUB	AWESUB			
HITEMP		COMP					
IBSUB		SEC3SB					
IMPEFF		COMP					
INPUT		E488M2					
INTGL		E488M2					
ITERP1		ACCEL	HITEMP	IMPEFF	ITERP2	LOTEMP	ONETEMP
		RSPNSE					
LIQUID		TCHEM					
LOOK2	E	AREAS	ELIPS				
LOOK3	E	AREAS	ELIPS				

Subroutines Cross Index (Continued)

Subroutine		Called by These Subroutines				
LOTEMP		COMP				
LP1SUB		PC1SUB	SEC2SB			
LP2SUB		PC2SUB	SEC1SB	SEC2SB		
LP3SUB		PC3SB	SEC1SB	SEC2SB		
LP4SUB		PC4SB	SEC2SB			
LRSUB		ASESUB				
MACHNO		NOZL				
MAIN						
MAINCO		TCHEM				
MATRIX		EQLBRM				
MODCLC		E488M2				
MTRCST		COMP				
NEWING		TCHEM				
NEWOF	E	ROCKET	SAVE			
NEWRAP		SETUP1				
NORMAL		TCHEM				
NOZINP		COMP				
NOZL		COMP				
NOZZSB		SEC1SB				
NREQ1		SETUP1				
NREQ2		SETUP1				
NREQ3		SETUP1				
NREQ4		SETUP1				
NREQ5		SETUP1				
NREQ6		SETUP1				
ONETEMP		COMP				
OUT1		RKTOUT				
OUT3	E	OUT1	RKTOUT			
PATSH		MAIN				
PCGSUB		PC2SUB				
PC1SUB		SEC1SB				
PC2SUB		SEC1SB				
PC3SUB		SEC1SB				
PC4SUB		SEC1SB				
PEPCSB		SEC3SB				
PROPST		COMP				
PTLSTB		E488M2				
RASUB		ASESUB				
RATESB		HITEMP	IBSUB	LOTEMP	ONETMP	SEC3SB
RATESB		INPUT				
RCSUB		AS2SUB	AS3SUB			
REACT		MAINCO				
RKTOUT		ROCKET				
ROCKET		MAINCO				
ROCKET1	E	ROCKET				
RSPNSE		E488M2				
RTCKSB		SEC1SB				
SAVE		ROCKET				
SBPHAT		STBINT				
SBQBAR		STBINT				
SEARCH		MAINCO				
SEC1SB		COMP				

Subroutine Cross-Index (Continued)

Subroutine		Called by These Subroutines				
SEC2SB		COMP				
SEC3SB		SEC2SB				
SETUP1		COMP				
SETUP2		COMP				
SETUP3		COMP				
SETUP4		COMP				
SETUP5		COMP				
STBCLO		CLOS	STBDAT			
STBDAT		SEC3SB				
STBINT		E488M2				
STBNOZ		NOZL	STBDAT			
STBS2		STBDAT				
TCHEM		COMP				
TRAJ		COMP	TRAJIN			
TRAJIN		COMP				
UBCALC		E488M2				
USERCS		COMP				
USEREF		COMP				
USERRB		HITEMP	IBSUB	LOTEMP	ONETMP	SEC3SB
USERRH		TCHEM				
USERSE		PROPST				
VOLUME		NOZL				
WACL1	E	CASEAN	CLOS			
WFCL1	E	CASEAN	CLOS			
WF2A3	E	CASEAN	CLOS			
XRSUB		ASESUB				

NOTES

(1) Supplementary notation "E" (e.g. "AFTCL1 E") indicates an alternate entry into the subroutine in the second column.

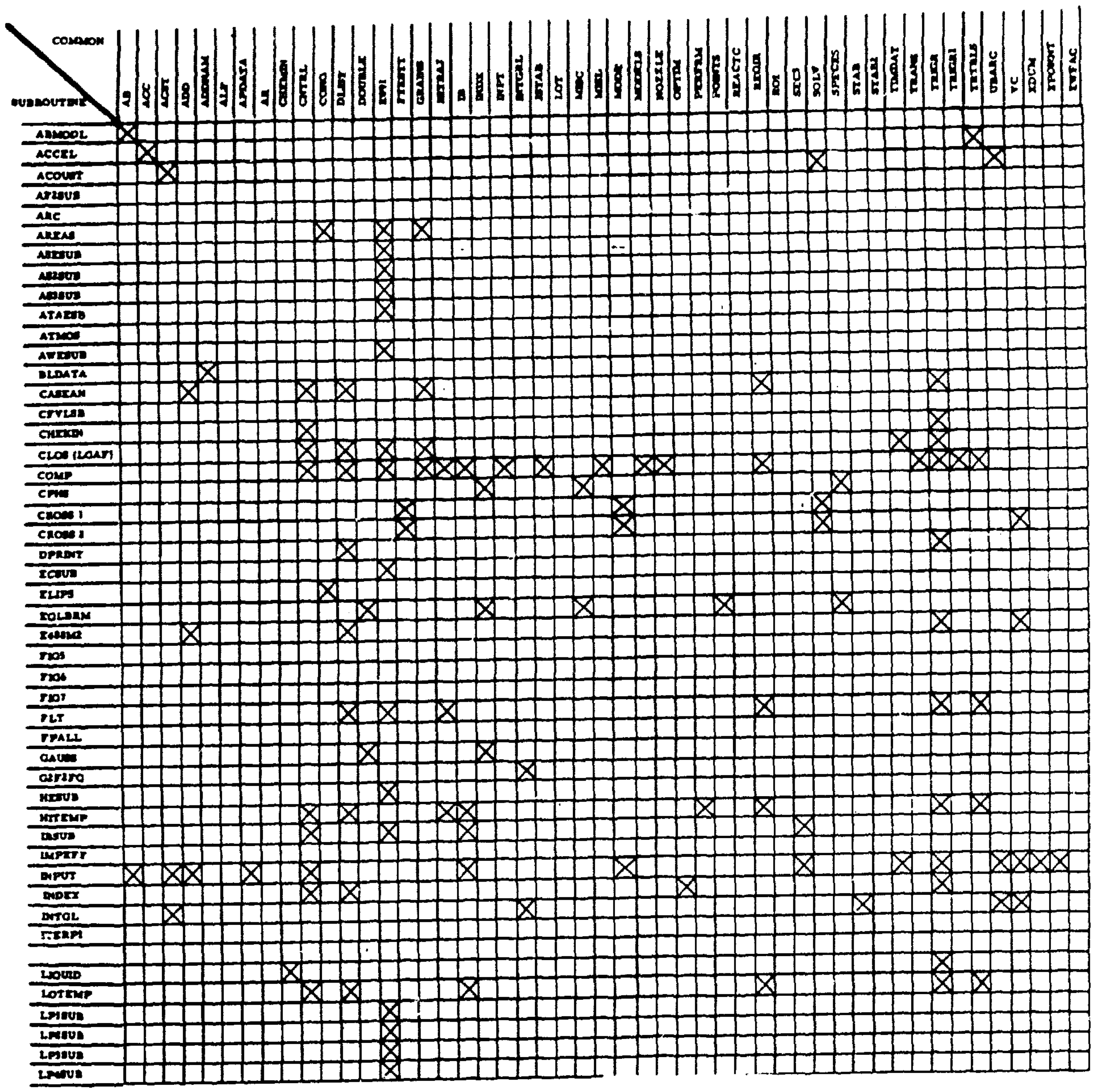
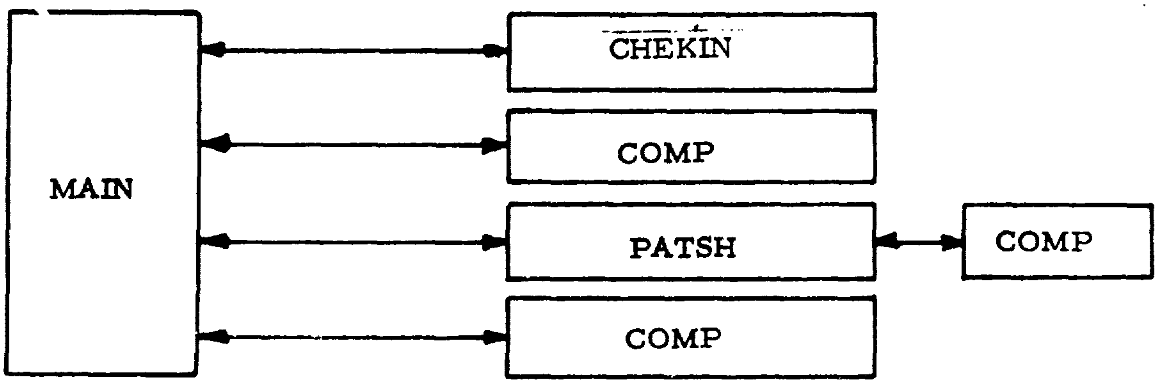


Figure 1. Subroutine - Common Statement Cross Index

Subroutine	AB	ACC	AGST	ADD	ADDRAM	ALF	APDATA	AR	CHEMIN	CNTRL	CONO	DLIST	DOUBLE	EM1	FTESTT	GRAINS	HSTRAJ	IB	INDX	INPT	INTGRL	ISTAB	LOT	MISC	MISL
LRBUR																									
MACHNO																									
MAINCO																			X					X	
MATRIX													X												
MODCLC			X																						
MTRCST																									X
NEWING					X																				
NEWRAP																									
NORMAL									X			X													
NOZINP										X		X		X											
NOZL										X		X													
NOZZSB														X											
NREQ1																X									
NREQ2																X									
NREQ3																X									
NREQ4																X									
NREQ5																X									
NREQ6																X									
NREQ7																X									
NREQ8																X									
NREQ9																X									
ONETEMP										X		X						X							
OUT1																			X						
PATSH																									
PCOSUB																									
PC1SUB														X											
PC2SUB														X											
PC3SUB														X											
PC4SUB														X											
PKPCSB																									
PROPST										X		X		X		X									
PTLSTB			X	X		X		X															X		
RASUB																									
RATESB																	X								
RCSUB														X											
REACT					X														X					X	
RKTOUT																			X						
ROCKET																			X					X	
RTCKSB														X											
RSPNSE	X		X	X		X	X	X																	
SAVE																			X					X	
SBPHAT			X																						
SBQBAR			X																						
SEARCH																			X					X	
SEC1SB														X								X			
SEC2SB														X											
SEC3SB										X		X		X				X							
SETUP1										X		X		X		X									
SETUP2										X		X		X		X									
SETUP3										X		X		X		X									
SETUP4										X	X	X		X		X									
SETUP5										X		X		X		X									
STBDAT										X				X											
STBINT			X																				X		
TCHEM					X		X		X	X		X													
TRAJ		X																							
TRAJIN		X										X													
VBCALC			X																						
USERCS																									X
USERRB																		X							
USERRF																									
USERRH																									
USERSE																									
VOLUME																									
XRSUB																									

Subroutine	MODE	MODELS	NOZZLE	OPTIM	PERFRM	POINTS	REACTC	RTQIR	ROI	STCS	SOLV	SPECIES	STAB	STAN	TIMDAT	TRANS	TRIGR	TRIGAI	TSTBLS	UBABC	VC	XDCM	XPOINT	ZVTAC
LRBUR																								
MACHNO																								
MAINCO						X						X					X							
MATRIX						X						X												
MODCLC	X										X										X			
MTRCST								X									X							
NEWING																								
NEWRAP																								
NORMAL																	X							
NOZINP			X														X	X						
NOZL			X		X										X	X	X							
NOZZSB																								
NREQ1																								
NREQ2																								
NREQ3																								
NREQ4																								
NREQ5																								
NREQ6																								
NREQ7																								
NREQ8																								
NREQ9																								
ONETEMP					X			X									X		X					
OUT1						X						X				X	X							X
PATSH				X																				
PCOSUB																								
PC1SUB																								
PC2SUB																								
PC3SUB																								
PC4SUB																								
PKPCSB																								
PROPST								X									X							
PTLSTB													X		X		X			X		X		
RASUB																								
RATESB										X							X							
RCSUB																								
REACT							X									X	X							
RKTOUT						X										X	X							
ROCKET						X										X	X							
RTCKSB																	X							
RSPNSE																				X		X	X	
SAVE												X												
SBPHAT																								
SBQBAR																				X				
SEARCH												X												X
SEC1SB																	X							
SEC2SB																	X	X						
SEC3SB								X		X				X			X	X	X					
SETUP1																	X							
SETUP2																	X							
SETUP3																	X							
SETUP4																	X							
SETUP5																	X							
STBDAT														X	X	X	X		X					
STBINT													X							X				
TCHEM							X								X	X								
TRAJ								X	X								X		X					
TRAJIN								X	X								X		X					
VBCALC																				X				
USERCS																								
USERRB		X								X														
USERRF																								
USERRH																								
USERSE																								
VOLUME																								
XRSUB																								

Figure 1. Subroutine - Common Statement Cross Index (Cont'd)



MAIN: Reads control inputs; initializes some parameters; controls printout; calls search routine

COMP: Executive subroutine passes information between subroutines; calculates some penalties and overall objective function (OBJ); provides printout

PATSH: Adjusts specified parameters; evaluates changes in objective function (OBJ)

Figure 2. Overall Code Organization

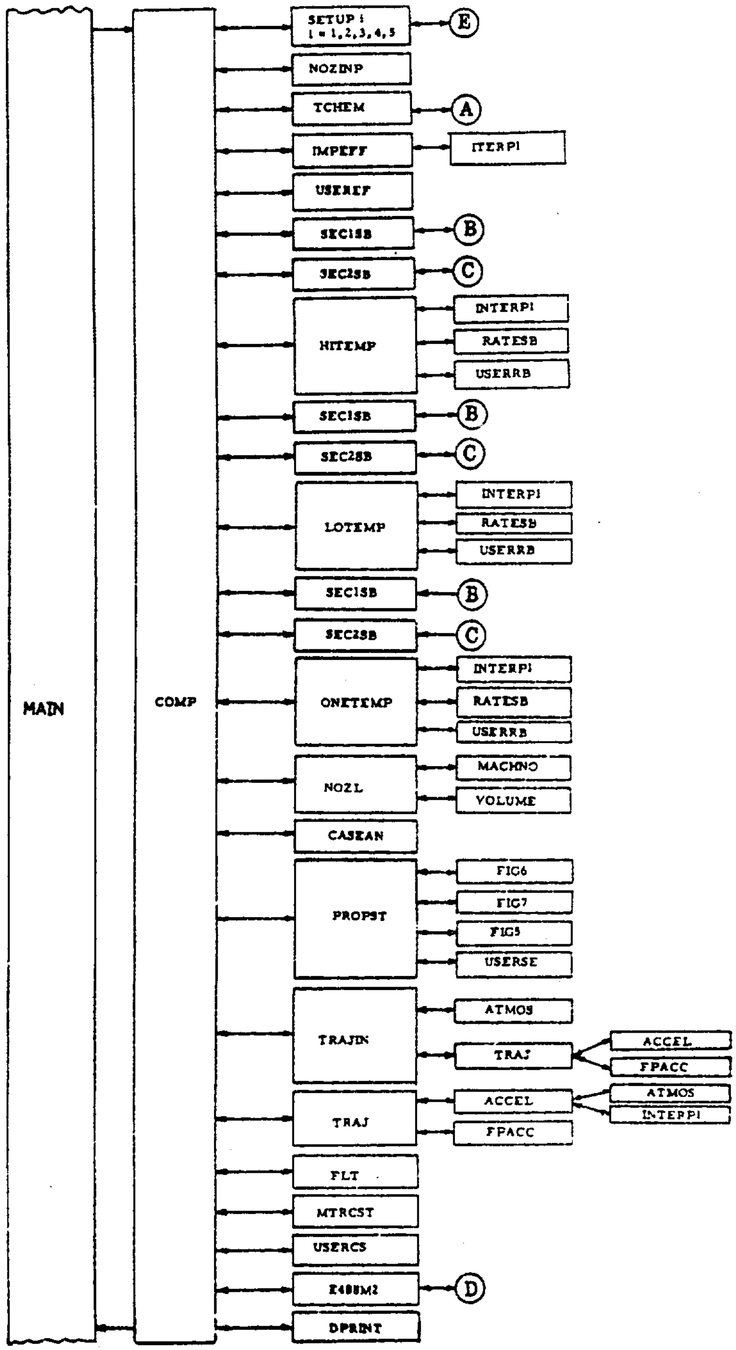


Figure 3. Subroutine COMP Flow Chart

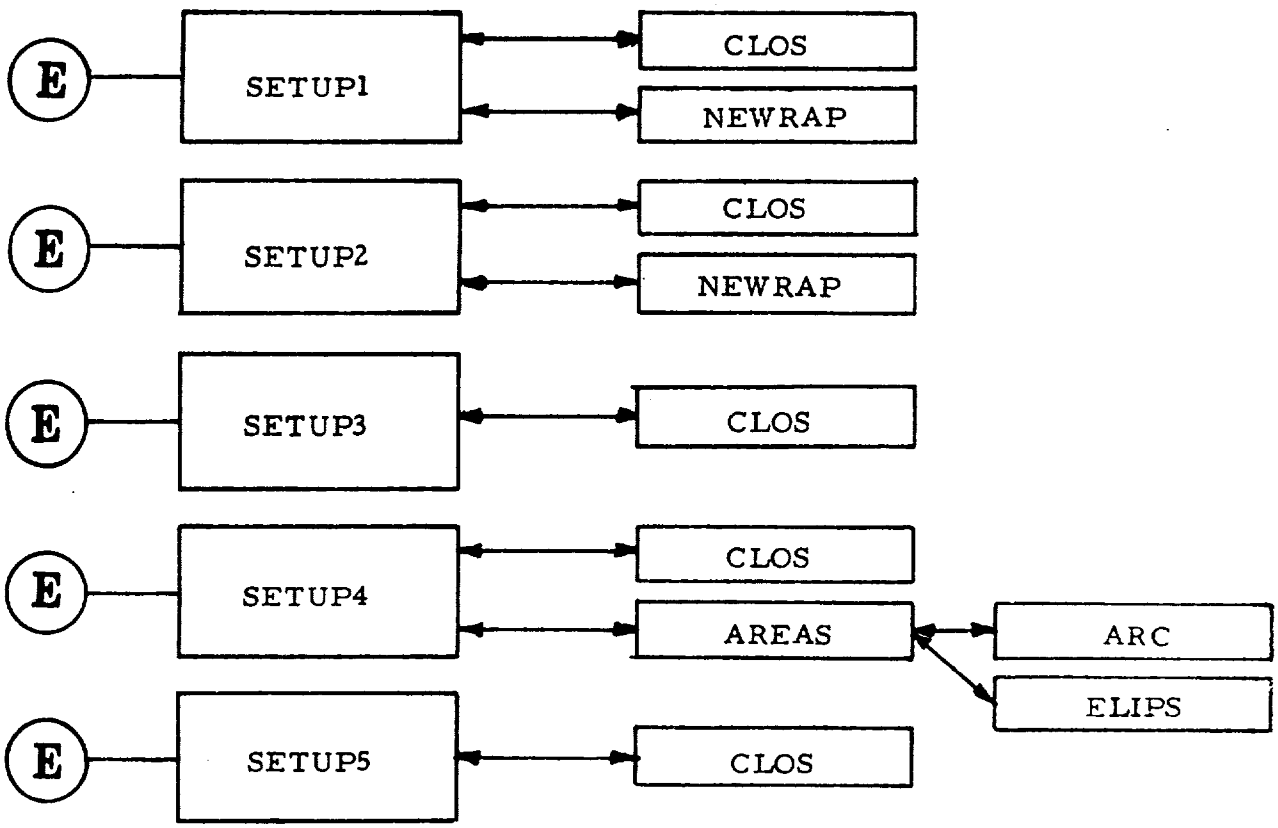


Figure 4. Subroutine SETUPi Flow Chart

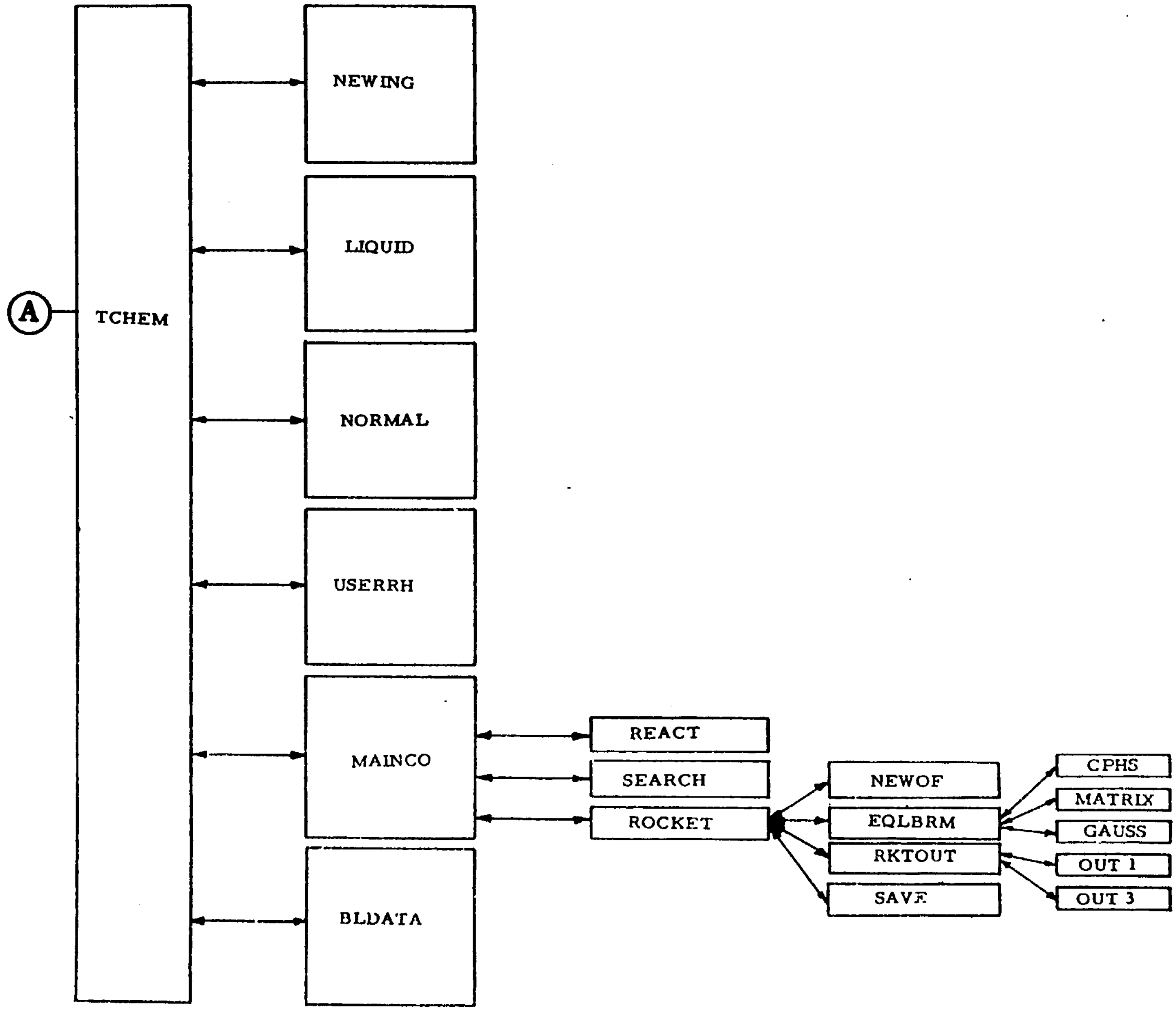


Figure 5. Subroutine TCHEM Flow Chart

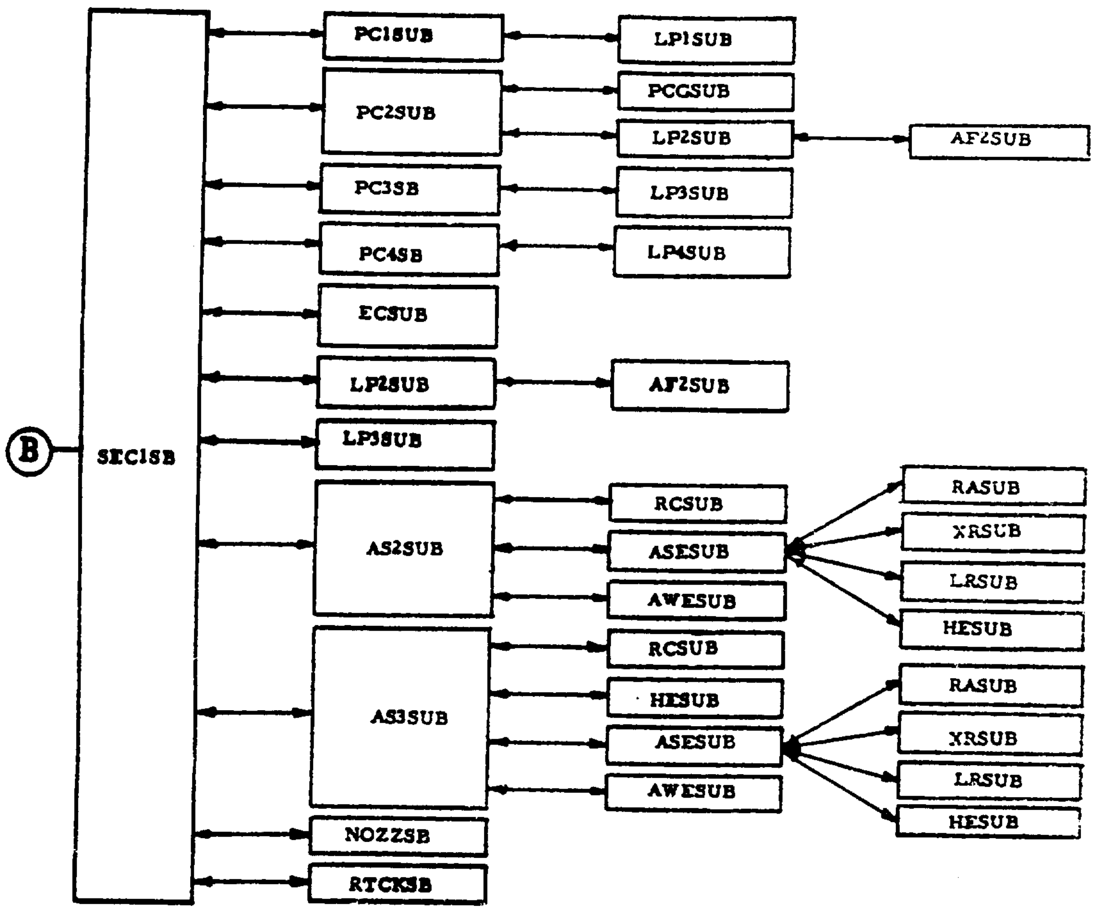


Figure 6. Subroutine SEC1SB Flow Chart

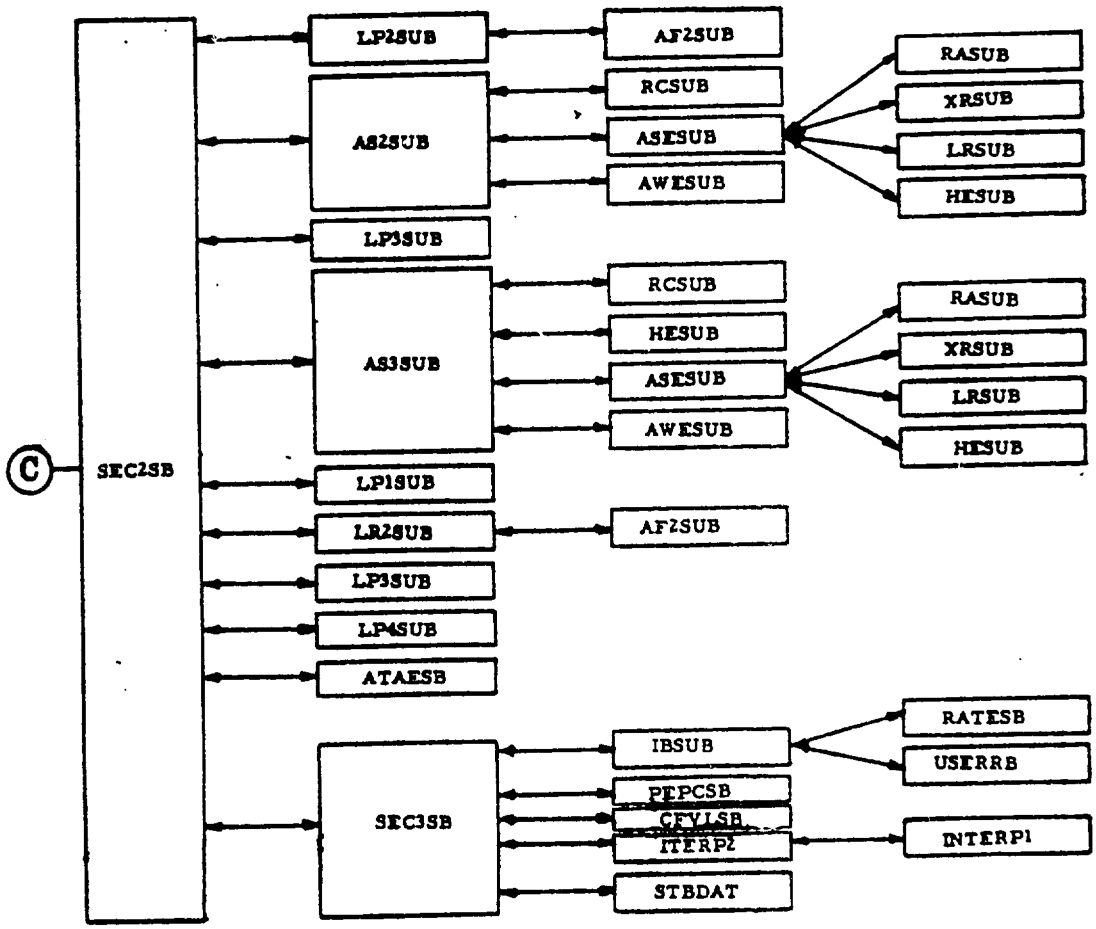


Figure 7. Subroutine SEC2SB Flow Chart

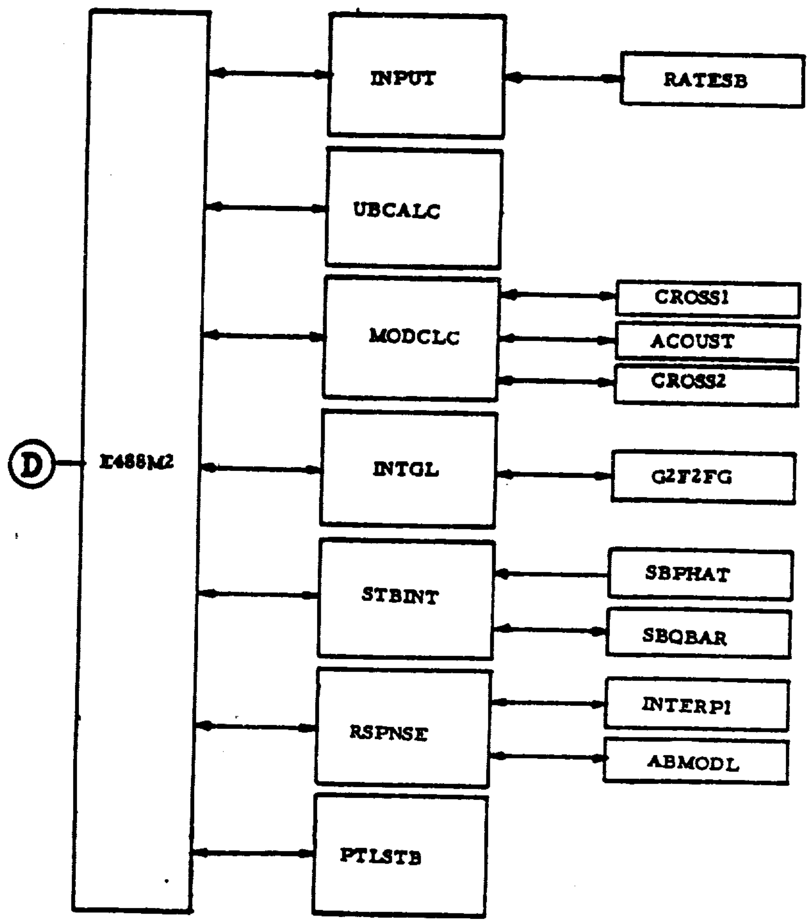


Figure 8. Subroutine E488M2 Flow Chart