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Users Manual For the LIMIT Code -

Hydrogen Analysis in Reactor Containments

Vincent P. Manno Michael W. Golay

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Energy Laboratory and Department of Nuclear Engineering Massachusetts Institute of Technology Cambridge, MA 02139

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Abstract

The LIMIT code is a new containment analysis code capable of simulating hydrogen transport events. The BEACON [1] code served as the foundation upon which LIMIT is built. The analytical aspects of LIMIT's features are documented in the work of Manno and Golay [2]. This document is the code users manual. It is assumed that the user also possesses the original BEACON code manual since both documents are required for code utilization.

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1.0 Introduction

The analytical modelling of hydrogen transport in reactor containment buildings is an important capability in nuclear safety assessment. The development and validation of a computer code that accomplishes this analysis is reported in the work of Manno and Golay [2]. The program, called LIMIT, is built upon the BEACON [1] containment analysis code. The basic code structure, input/output form and computer-related characteristics were slightly modified in order to make effective use of the existing BEACON documentation. As such, this document is structured assuming the original BEACON manual is also available.

Section 2 provides an itemized commentary on each of the original manual's sections with information relating to its applicability given LIMIT's capabilities. The commentary on Chapter 4 - Program Application is particularly important to the user since revised input/output formats are specified. Section 3 of this work addresses job control language (JCL) issues and supersedes the analogous discussion of the original manual. (The user is cautioned that code modification requires a detailed familiarity with CDC system capabilities.) Finally, Section 4 details input data and code results for a few sample problems. The revised code remains capable of handling the sample problems reported in the original manual with minor input deck modification.

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2.0 Revisions to the BEACON Users Manual for Hydrogen Analysis

Despite the major differences between LIMIT and BEACON, the original users manual remains applicable if the revisions described in this section are noted. The changes of greatest interest to the user are the new analytical capabilities which are documented elsewhere and input/output requirements which are specified herein. The format of this section is to comment on each subsection of the original manual.

- **1.** Introduction Clearly this section is not descriptive of the revised code capabilities.
- 2. Program Overview Table 2 is not complete especially in the areas of hydrogen analysis, enhanced numerical techniques, revised thermodynamic modelling and proqramming features. The overall computational logic sequence of Figure 1 remains valid.
- 3. Model Descriptions Reading this section in conjunction with Chapter 3 of Reference 2 provides a complete picture of available models.

3.1 Eulerian Region Modelling - Multicomponent, nearly incompressible longer term model is now also an option.

3.1.1 Numerical Technique - Section 3.3.4 of Reference 2 describes the new numerical schemes introduced.

3.1.2 Coordinate Systems - The slower mixing analysis (only) includes a full three dimensional modelling capability.

3.1.3 Variable Mesh Spacing - no substantive change.

3.1.4 Boundary Modelling - The information provided remains correct but section 3.3.4 of Reference 2 should be consulted for boundary model options of the slow mixing equation set.

3.1.5 Obstacle Cells - no substantive change.

3.1.6 Restricted Flow Modelling - no substantive change.

3.1.7 Mass, Momentum and Energy Sources - Hydrogen is now an additional source material as described in section 3.2 of Reference 2.

3.1.8 Form and Friction Losses - no substantive change.

3.2 Mixed-Dimensional, Multiregion Modelling - The three-dimensional option of the slower mixing model is limited to single region problems.

3.2.1 One Dimensional Flow Modelling - The new slower mixing equation set is also applicable to one dimensional regions.

3.2.2 Lumped Parameter Modelling - Section 3.2.2 of Reference 2 describes the inclusion of hydrogen conservation in the original lumped parameter formulation as well as an improved lumped parameter model based on a true junction-node formulation.

3.2.3 Coupling Methods - No changes in either the spatial or temporal computational coupling logic except as noted earlier in regard to 3-D models.

3.3 Wall Film and Heat Structure Modelling - The capabilities of the code in these areas are extended to be more useful in long term simulations. The user is cautioned against using the film option in conjunction with the new mixing model due to its unrequired complexity and the computational effort involved. The heat structure modelling remains relatively intact but the heat transfer correlation package has been improved.

3.4 Thermodynamic Modelling - A new equilibrium thermodynamic model based cn the assumptions of incompressible liquid and perfect gas-like gaseous components coexiting is utilized by the MITHYD subcode.

3.4.1 User-Defined Interphasic Exchange Functions - These models are only appropriate for rapid two-phase blowdown transients, if at all. The so-called "best estimate" option is the only encoded choice appropriate to any problem involving a non-condensible gas such as air or hydrogen.

3.4.2 Best-Estimate Interphasic Exchange Functions - see discussion of 3.4.1 above.

3.4.3 Equation of State - In addition to the comments presented in reference to 3.4, the user should note that the BNL equation of state option has not been modified for the inclusion of hydrogen due to the drawbacks of this scheme documented in this section.

3.4.4 Transport Properties - The molecular thermal conductivity and dynamic viscosity of hydrogen have been included as discussed in section 3.2.3 of Reference 2. Treatment of molecular mass diffusivities has also been addressed in the MITHYD subcode.

4.0 Program Application - These changes relate to the actual utilization of the code.

4.1 Input Description - The major changes in this area involve the modification of existing input cards and the addition of new ones.

4.1.1 General Information - Table 3 is of limited value since it describes older versions of the original code. The format specification, however, remains unaltered.

4.1.2 Basic Input Data - Only modified or new cards are documented below. All variables marked with an asterisk refer to 3-D input data.

00110 Card - modified

W9-I JSLOW* Problem solution selector

- -1 **-** only modified BEACON two phase flow model is used for continuum solution,
- O **-** either modified BEACON or MITHYD (2-D option only) may be employed using SWITCH parameter for internal decision,
- 1 **-** MITHYD (2-D option) used for continuum solution,
- 2 **-** lumped parameter run using new node/junction model formulation,
- 3 MITHYD only in either a 3-D Cartesian or 3-D "incomplete cylinder" geometry. Single region problems only.
- 4 MITHYD only in a complete 3-D cylindrical geometry. Single region problem only.
- W10-R SWITCH Switching criterion for change from BEACON model to MITHYD in a particular spatial domain. Used only with JSLOW = **0.** Only a single uni-directional transition is allowed for each mesh. SWITCH is the maximum cellwise fractional density change.

00145 - modified

Indices of particular parameters are different and Table 2.1 is used to specify input for this card (valid for 2-D options only).

Table 2.1 Cell Variable Index **(AASC** array)

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Table 2.1 Cell Variable Index (AASC array)(cont'd)

Notes:

 1 cell variable only used by modified BEACON equation set

 $\Delta \phi$

 $\sim 10^6$ $\sim 10^{-10}$

 2 no longer used

 3 may have somewhat different definition depending upon model used $43-D$ only

 $\sim 10^{11}$ km $^{-1}$

00150 - modified

Plotting option is not operational at this time, therefore omit 00150.

00200 - modified

LMAX has the meaning specified in relation to the modified BEACON equation set. When MITHYD is employed, LMAX is the number of calculational cycles before the reference state is updated. Specification of a very large number for LMAX will inhibit reference state update. See discussion of 3.3.4 of Reference 2 for more information.

00240 - modified

EOSOPT = LASL is the only valid option for this code.

00301 to 00399 - modified

OPK definition should be based on Table **A.1.**

00400 - new card - Slow Mixing Parameters (required)

W3-R RELAX Successive over-relaxation parameter used in SMAC iteration, $(0.5 < RELAX < 2)$. Suggested value = 1.8 .

- W4-R SCHMS Turbulent Schmidt number for steam (suggested $value = 1.0$).
- $W5-R$ SCHMH H₂ turbulent Sc#. (Suggested = 1.0)
- $W6-R$ SCHMA Air turbulent Sc#. (Suggested = 1.0)
- W7-R SCHML Liquid turbulent Sc#. (Suggested **<<** 1.0)

default values 0 1.0 1.0 1.0 1.0 1.0 1.0

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00410 **-** new card **-** Turbulence Model Constants (required)

- W1-R CMU Coefficient relating E, TKE, **E** and **VT.** Suggested = 0.090) If CMU ≤ 0.0 , turbulence equations are not solved, $i.e.$ completely laminar assumption.
- W2-R CSIG1 Coefficient of shear production term in **E** equation. (Suggested = 1.44)
- W3-R CSIG2 Coefficient of $\rho \xi^2 / TKE$ in ξ equation. (Suggested **=** 1.92)
- W4-R CSIG3 Coefficient of buoyant production term in **E** equation. (Suggested **=** 1.44)
- W5-R SIGT Turbulent Prandtl number. (Suggested **=** 0.9) If SIGT $>$ 100.0, energy equation is not solved, T.e. isothermal flow assumed.
- W6-R SIGK TKE turbulent Prandtl number. (Suggested = 1.0)
- W7-R SIGS Dissipation turbulent Pr number. (Suggested **=** 1.3)
- 0042C new card Molecular Mass Diffusion (required)
	- W1-I IDIF Either constant input mass diffusivities used (= **0)** or dynamically calculated multicomponent diffusivities used **(=** 1).
	- $W2-R$ DMS Steam molecular diffusivity (m^2/sec)
	- W3-R DMH Hydrogen molecular diffusivity
	- W4-R DMA Air molecular diffusivity
	- $W5-R$ DML Liquid molecular diffusivity (suggested = 0.0)
- **0500 -** new card Blower Cell Model (optional, see 4.3.2 of [2])

W1-I NBLOW Number of blower cells (10 maximum)

- 05XO new card Location of Blower Cell X
	- W1-I **Ii** Radial index of cell
	- W2-I J1 Axial index of cell
	- W3-I K1* Azimuthal or depth index of cell
	- W4-I IREAD Number of tabular data points (9 maximum)
- W1-R TIME Time (sec)
- W2-R BLAIR Air density (kq/m^3)
- W3-R BLHYD Hydrogen density $\text{(kg/m}^3)$
- W4-R TEMP Temperature (K)
- $W5-R$ FLOW Volumetric flow (m^3/sec)

M1000 card - modified

- $W10-I$ ISLOW =0, switching logic used in conjunction with $JSLOW=0$ option applicable to this mesh or $=1$, MITHYD only.
- W11-R ROREF Initial mesh reference density
- W12-I KBAR* Number of interior cells in third dimension. Set to 1 for 2-D runs.
- W13-R DTHCON* Cell dimension in third dimension.

M1010 Card - modified

If no slip boundary condition is used in conjunction with the turbulence model, wall-shear generated turbulence as per the modified law of the wall is included for the r and z directions. This option is not recommended unless a very fine mesh nodalization is employed.

- W5-A NSIDE* North side (positive theta direction) slip indicator
- W6-A SSIDE* South side slip indicator
- M1040 new card Third Dimension Variable Nodalization (optional)
	- $W(1)$ -R DTHTAB (1) * Theta mesh increments, either in units of length specified on
	- W(KBAR)-R DTHTAB(KBAR)* M1010 for Cartesian coordinates or fraction of a circle for cylindrical coordinates. Note for cylindrical coordinates, the sum of DTHTAB(K) should not exceed 1.0 (i.e. more than a full circle,).

M1101-M1199 Cards - modified

FLUID = HYD (i.e. Hydrogen) is a valid entry.

W12-R XHYD Initial hydrogen mass fraction in gas field

- **W13-I** KXI^* Initial θ -direction cell index (=2 for 2-D)
- W14-I KXF* Final θ -direction cell index (=2 for 2-D)
- M1201-M1299 Cards modified
	- W9-R TKEIN Initial TKE level (m^2/sec^2)
	- W1O-R DISIN Initial dissipation level (m^2/sec^3)
	- **W11-I** KXI* Initial K index
	- W12-I KXF* Final K index

W13-R WGIN* Initial third dimensional velocity

M1401-M1499 Cards - modified

W6,7-I KXI*,KXF* Theta indices for obstacle definition

M1601-M1699 Cards - modified

Analogous changes to M1101-M1199 cards

M1701-M1799 Cards - modified

 $W5-R$ TKEIN Inflow TKE level (m^2/sec^2)

W6-R DISIN Inflow dissipation level (m^2/sec^3)

W7-R WGIN* Inflow theta velocity

L2010 Card - modified

FLUID = HYD (i.e. hydrogen) is a valid option

W7-R XHYD Initial mass fraction of hydrogen in gas field

2960+50S Card - modified

SUBST **=** HYD (i.e. hydrogen) is a valid option KSTAR* Theta source cell index

W13-R PHI* Angle of source velocity in theta direction measured from vertical in a clockwise direction

9001-9050 - new cards - Lumped Parameter Junction Data (optional) W1-I NJN Junction number W2-I IFR Upstream lumped parameter zone W3-I ITD Downstream lumped parameter zone $W4-R$ XKF¹ Forward loss coefficient $(1/m⁴)$ $W5-R$ XKF¹ Reverse loss coefficient $(1/m⁴)$ $W6-R$ XIN^2 Junction inertia (1/m) XKF=XKR = K/2A $_3^2$ where A_i= junction flow area and K = nominal'loss coefficient $2XIN = L/A$ where L = effective flow length, A = effective flow area Note: Up to 50 such junctions may be specified. These data are only used if JSLOW = 2 on Card 00110. Also, one dummy continuum region must be included in the input deck.

1YY0009 Card - changed

New options for best estimate containment heat transfer models have been added as specified in the following table. The natural convection options are recommended since they seem to fall within the range of most available data. For each case laminar or turbulent flow conditions are dynamically determined depending upon local conditions. The "local" vs. "average" options differ in the treatment of cell conditions as they affect the overall heat transfer coefficients. The local option is most accurate.

NEW OPTIONS INTERNAL FLAG (CONTYP) COMMENT

4.2 Output description - The printed output format is essentially the same as that described in the manual with a few specific alterations which are detailed below. The plotting options have been removed due to hardware and software differences between the mainframes used at INEL and the CYBER-176 machine. Major compatibility problems in the area of system-specific software invoked by the INEL Environmental Library seems to be the major problem area.

4.2.1 Print Output - The changes to the print output are related to listing new parameters which were not used in the original code.

4.2.2 Plot Output - This is not a valid option at this time.

4.2.3 Postprocessed Plots - This is not a valid option at this time.

4.3 Tape Restart - The restart option has been modified to allow proper restart of the new code. The user should permanently store the restart output file (TAPE4) and access it as the input restart file (TAPE3) of the subsequent job. See section 3 of this work for more information.

4.4 User Guidelines - The guidance of this section remains valid save for the following modofications.

4.4.1 Nodalization - no substantive changes.

4.4.2 Multiregion coupling - no substantive changes.

4.4.3 Gravity - no substantive changes.

4.4.4 Boundary Conditions - see previous card specific instructions.

4.4.5 Iteration Converence Criteria - EPSG is used as the convergence criterion of the MITHYD subcode. LMAX has the dual definition described in the previous discussion of Card 200.

4.4.6 Timestep Advancement - As the discussions of section 3.3.4 and Chapter 4 of this work indicate, the time step limitation of the MITHYD is less restrictive than the BEACON formulation (i.e. XDTC **+** 1.0).

4.4.7 Numerical Instability - These remain valid guidelines with the additional caution that feedback from the energy equation to the momentum equation in MITHYD could cause convergence problems due to nonphysical density field solutions.

4.4.8 Input and Output - no substantive changes.

- 5.0 Sample Problems The new code is capable of handling any of these problems save for the plotting options and some minor input deck changes to accommodate the revised input cards.
- 6.0 Program Structure The modifications described here can be better understood if they are studied in conjunction with Chapter 3 and Appendix A of Reference 2.

6.1 General - The remarks of this section remain approximately accurate. Small core memory required has increased approximately 15% from the original code. Segmentation loading is discussed in the next section and Appendix A of Reference 2.

6.2 Dynamic Storage Allocation - In order for the user to better appreciate this section the INEL Environmental Library Manual [3] and CDC-specific software documentation must be consulted. Each computational cell now requires 83 words of storage (total of 115 with 32 overwrites). This increase in variables per cell had led to a computational cell limit of 1580.

6.3 Subroutine Descriptions -The new subroutines are briefly described below. The modifications and deletion of existing routines is addressed in Appendix A of Reference 2.

6.3.1 Main Program and Control Subroutines - no additions or deletions.

6.3.2 Fluid Region Input Subroutines

SLOINP **-** New subroutine using INP2 to read cards 400 to 420.

6.3.3 Heat Structure Input Subroutines - No additions or deletions.

6.3.4 Plot and Print Output Subroutines - The following plotting subroutines are deleted - PLOTS, PPLOTS, VPLOTS, CPLOTS, FLMPLT, FLMPLTB, POBPLT, ADV, OCPLT, FIXLBL, FRAME, PLT AND DRV.

6.3.5 Fluid Dynamics Computations Subroutines

- ADISLV **-** General ADI solution scheme solver.
- AIJ $-$ Evaluates $A_{i,j}$ of transport equations solutions.
- BIJ Evaluates **Bij.**
- BLOINP **-** Processes blower cell input.
- BLOWER **-** Updates blower cells.
- $CRIJ -$ Evaluates C_{11}^r .
- CTIJ Evaluates C_{1i}^{θ} .
- CZIJ Evaluates **Cij.**
- DEXPL Evaluates explicit change in transported entity. Also applies non-zero divergence correction.
- DFNADI General solution routine for four mass transport equations.
- DIFCAL Calculation of cell specific mass diffusion constants.
- DIJ Evaluates D_{ij}.
- $\overline{\mathcal{L}}$ EIJ - Evaluates E_{ij}.
- FIJ **-** Evaluates **Fij.**
- GIJ Evaluates G_{ij}.
- ENADI **-** General energy equation solution.
- MITHYD **-** Overall controlling routine analogous to KFIXT of BEACON
- MOCSLV **-** Lagrangian treatment of convection routine.
- PITER Pressure/velocity iteration portion of SMAC solution.
- **SAVCQQ -** Saves n-level variable values in case MITHYD time step requires reduction due to compressibility check.
- SWTCH **-** Subroutine containing logic to decide whether switch from modified BEACON to MITHYD is desirable.
- TILDEM **-** Explicit portion of momentum equation solution.
- TRBADI General solution routine for turbulence equations.
- TRBSRC Evaluates production terms of TKE and disipation equations.
- UPDATE Multifunction routine including calculation of various parameters such as hydrogen volume fraction, decision logic for time step reduction and reference state updating. Also includes thermodynamic state model.
- VNCONV **-** Evaluates non-convective terms of momentum equation.

6.3.6 Mixed-Dimensional Coupling Subroutines - no additions or deletions.

6.3.7 Wall Film Computations Subroutines - no additions or deletions.

6.3.8 Heat Structure Computations Subroutines

HTNEO **-** New heat transfer package.

6.3.9 Equation of State Subroutines

SATVAP - Curve fit of saturated vapor density vs. temperature.

SLOCG - Evaluates mixture specific heats.

6.3.10 Auxiliary Subroutines - no additions or deletions.

6.4 Implementation Requirements - There are substantial differences between **COC** operating systems. The Job Control Language (JCL) described in section 3 is valid for use on a CDC CYBER-176 machine under a NOS operating system. The user should consult the proper CDC documentation if code modification or novel installation is required. Specific JCL for various possible running modes are discussed in Appendix C of this work. Running time is discussed in Chapter 4 of Reference 2.

7.0 References - no substantive changes.

Appendix A - Governing Equations and Numerical Procedures

and

Appendix B - Best Estimate Interphasic Exchange Functions

These appendices remain valid subject to the discussions of Chapter 3 of Reference 2.

Appendix C - Time History Plot File Program - is not applicable at this time.

This code is structured to be run on a CDC CYBER-176 machine under a NOS Operating system. Direct use on any other system may involve a substantial conversion effort given that the program utilizes many unique CDC features such as segmented loading, dynamic storage allocation and update format. The job control language (JCL) specifications presented address three possible utilization modes production, modification and restart. Production and restart mode execution can be accomplished without detailed user familiarity with CDC-based software. Modification and testing however demands knowledge of many software systems. The most useful documentation for performing code modification are the NOS Reference Manual Set [4], UPDATE Utility Manual $[5]$, LOADER Manual $[6]$ and X-EDIT Manual $[7]$.

The subsequent JCL discussions assume the user is utilizing a magnetic tape with the contents depicted in Table 3.1 and permanent disk space which includes various data files such as input data decks and update editing directives. If reasonably-priced disk space is available, magnetic tape use can be entirely eliminated.

3.1 Production Mode

Figure 3.1 presents a sample job for a production mode run. The first card is a job card. The second specifies job name, running time limit and priority. The next two are charge cards. The REQUEST statement mounts the tape which is assumed to be an unlabelled 9-track tape designated LL0364. The next seven instructions copy the first

Table 3.1: Sample Magnetic Tape Contents

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Figure 3.1: Sample Production Mode JCL

/JOB EXEJOB,T200,P2. /USER /CHARGE REQUEST,TAPE,VSN=LLO364,LB=KU,NT,PO=W. COPYBF,TAPE,ENLOBJ. COPYBF,TAPE,CODEOBJ. COPYBF,TAPE,SUBLIB. COPYBF,TAPE,SEGCRD1. COPYBF,TAPE,DATA. REWIND,TAPE,ENLOBJ,CODEOBJ,SEGCRD1,DATA,SUBLIB. RETURN,TAPE. CALL,FTN176. RFL,CM=300000,EC=400. $REDUCE(-)$. SEGLOAD, I=SEGCRD1. LDSET,LIB=SUBLIB. LOAD,ENLOBJ,CODEOBJ. EXECUTE,BEACON,DATA,PL=50000. STIME. ROUTE,OUTPUT,DEF,CD=PR,UN=BTECHBB,ST=ECY. DAYFILE,L=FILEOUT. SAVE,FILEOUT. EXIT. STIME. ROUTE,OUTPUT,DEF,CD=PR,UN=BTECHBB,ST=ECY. DAYFILE,L=FILEOUT. SAVE,FILEOUT.

five tape files to local files of the names shown, rewinds the files and dismounts the tape. The CALL statement initializes the FORTRAN compiler. The next two statements define large and small core memory (LCM and SCM) allocation limits. The SEGLOAD card prescribes the segmentation loading pattern using the directives of file SEGCRD1. SEGCRD1 as well as the loading pattern produced by it are shown in Figure 3.2. The LDSET statement loads the compiled subroutines contained in NEWLIB. The next two statements load the environmental library and main code object files and execute the program using DATA as input data. The remaining instructions save the dayfile and route the output to the desired printer. The routing specifications are user-specific.

3.2 Modification and Testing

Code modification and testing involves detailed programming considerations. A general illustrative framework is provided here but successful implementation requires the accrual of significant user experience and expertise. The first sample JCL is provided in Figure 3.3 and assumes the user has formulated an update input file, called HYDUP, which specifies changes to particular subroutines. This job creates a compiled subroutine library which includes object code of all subroutines but not the main program in a library format. The first difference from the execution job is the use of the program library UPDATPL rather than the object code stored in MAINOBJ and SUBLIB. A Full Update is performed in which the entire code is included in the compile file. Hence the compilation defined by the FTN command involves the entire code (usually about 400 CPU seconds).

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Figure 3.3: Sample Modification JCL Assuming Subroutine

```
Library Does Not Exist
/JOB
MODJOB,T1000,PL.
/USER
/CHARGE
REQUEST,TAPE,VSN=LLO364,LB=KU,NT,PO=W.
COPYBF,TAPE,ENLOBJ.
SKIPF,TAPE,2.
COPYBF,TAPE,SEGCRD1.
COPYBF,TAPE,DATA.
COPYBF,TAPE,UPDATPL.
REWIND,ENLOBJ,SEGCRD1,DATA,UPDATPL,TAPE.
GET,HYDUP.
UPDATE,F,I=HYDUP,L=1,C=COMP,P=UPDATPL,N=NEWPL.
REWIND,COMP,NEWPL.
CALL,FTN176.
RFL,CM=300000,EC=400.
FTN,I=COMP,OPT=2,R=O,L=OUTPUT,SL=O,B=SUBOBJ,A,STATIC.
REWIND,SUBOBJ.
COPYBR,SUBOBJ,MAINOBJ.
COPYBF,SUBOBJ,LIBOBJ.
REWIND,LIBOBJ.
LIBGEN,F=LIBOBJ,P=NEWLIB.
REWIND,NEWLIB,MAINOBJ.
SKIPF,TAPE,10.
COPYBF,NEWPL,TAPE.
COPYBF,NEWLIB,TAPE.
COPYBF,MAINOBJ,TAPE.
REWIND,TAPE,NEWLIB,MAINOBJ.
RETURN,TAPE.
REDUCE(-).
SEGLOAD,I=SEGCRD1.
LDSET,LIB=NEWLIB.
LOAD,ENLOBJ,MAINOBJ.
Repeat last 10 lines of execution JCL.
```
The object file created includes the main program as the first record. Since that cannot be included in the subroutine library to be created, it is copied to a separate file MAINOBJ while the remaining subroutines are stored in LIBOBJ which is used to generate the NEWLIB library. The newly created program library NEWPL (analogous to **UPDATPL),** NEWLIB and MAINOBJ are then stored on the tape as the eleventh through thirteenth files, respectively.

The reason for generating a separate subroutine library is to allow more economical future modification. With an existing subroutine libary, future update runs need only involve selected subroutines. The compiling effort therefore is limited. For example recompiling a few subroutines may use 10-20 CPU seconds as opposed to the 400 CPU seconds for a full recompilation. The newly compiled subroutines are inserted into the existing subroutine library using a LIBEDIT command. Before the LIBEDIT command can be invoked the old subroutine library must be cast in a relocatable record format through a GTR command. The new subroutine library is generated from the output of the editing process. A sample job illustrating this approach is shown in Figure 3.4. The tape is assumed to contain files 9 through 11 generated by the first modification job. In addition, the user is assumed to have already available in permanent disk space, properly formulated Update directive file, HYDUP1, and library editing directive file LIBIN. This job replaces the old program library and subroutine library with the new ones cr eated by UPDATE and LIBGEN respectively. Note the Normal (not Full) Update mode is used.

- 30 -

/JOB

MODJOB1,T1000, P2.

/USER

/CHARGE

REQUEST,TAPE,VSN=LLO364,LB=KU,NT,PO=W.

COPYBF,TAPE,ENLOBJ.

SKIPF,TAPE,1.

COPYBF,TAPE,SEGCRDI.

COPYBF,TAPE,DATA.

SKIPF,TAPE,5.

COPYBF,TAPE,OLDPL.

COPYBF,TAPE,OLDLIB.

COPYBF,TAPE,MAINOBJ.

REWIND,TAPE,ENLOBJ,SEGCRD1,DATA,OLDPL,OLDLIB,MAINOBJ.

GET,HYDUP1.

UPDATE,I=HYDUP1,L=1,C=COMP,P=OLDPL,N=NEWPL.

REWIND,COMP,NEWPL.

CALL,FTN176.

RFL,CM=300000,EC=400.

FTN,I=COMP,OPT=2,R=O,L=OUTPUT,SL=O,B=SUBOBJ,A,STATIC.

 \cdot

REWIND,SUBOBJ.

GTR(OLDLIB,TEMP)REL/*

REWIND,TEMP.

GET,LIBIN.

LIBEDIT,B=SUBOBJ,P=TEMP,N=NEWOBJ,I=LIBIN.

LIBGEN,F=NEWOBJ,P=NEWLIB.

REWIND,NEWLIB.

Repeat last 20 lines of first modification job.

The code's restart capability is invoked by the use of BEACON input card 00105. The code reads input information from I/0 unit 3 and therefore an existing file named TAPE3 must be available before execution. The code generates restart data on I/0 unit 4 and hence after execution TAPE4 must be permanently stored. The exact details of this restart data storage and retrieval is user-specific.

4.0 Test Problems - Input Data Decks and Results

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Three sample test problems are described in this section which are useful for code installation debugging and gaining user experience. The rapid mixing equation set, slower mixing model and lumped parameter option are each tested by these simulations. The input and output of these problems are included on the LIMIT transmittal tape. More complex simulations are reported in Reference 2.

Rapid Hydrogen-Water Flow Into A Compartment

This first problem is a variation on a sample problem reported in the original BEACON manual. The general problem geometry is presented in Figure 4.1. The scenario involves a single compartment geometry with prescribed boundary conditions. The inlet flow is 50% hydrogen and 50% water (by volume) mixture which enters the lower left entrance region at a velocity of 3.048 m/sec. The initial compartment conditions are a stagnant mixture of 90% air and 10% water. An 11x14 uniform Cartesian continuum geometry is used in conjunction with the modified BEACON equation set (JSLOW = -1). A complete input data deck specification is provided in Figure 4.2.

The predicted hydrogen concentration profile and velocity field at 0.1 and 0.2 second into the simulation are shown in Figures 4.3 and 4.4. A plot of the hydrogen volume fraction time histories and five selected calculational locations (see Figure 4.1) are presented in Figure 4.5. The total CPU execution time on a CYBER-176 machine is 650 seconds for this problem.

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50% H_2 / 50% LIQUID

FIGURE 4.1: RAPID TRANSIENT SAMPLE PROBLEM DESCRIPTION

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 $\label{eq:2.1} \mathcal{L}(\mathbf{z}) = \mathcal{L}(\mathbf{z}) + \mathcal{L}(\mathbf{z}) = \mathcal{L}(\mathbf{z}) + \mathcal{L}(\mathbf{z})$

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 $\mathcal{L}^{\text{max}}_{\text{max}}$ and $\mathcal{L}^{\text{max}}_{\text{max}}$

83/25. EU LEGAL AUDU PROGRAM DATA **-** 35- + INPUT FILE FOR SAMPLE PROBLEM I 00100 ' MODIFIED BEACON SP2 WITH H2 INFLOW ** -ASIC PROBLEM INPUT 00110 0.0 0.2 0.001 SEC 10.0 1 NOXEG USERDEF -1 1.OE+!O **0012C** 0.02 **0.2** 00130 AUTODT 1 0.1 1.5 1.OE1O 00140 PRINT NOPRINT PRINT NOPRINT NOPRINT 00220 1 i. 0E4 *0.0* 0.0 0.0 *00230* 0 0.0 0.0 1.0E4 00240 LASL PT LBF/IN2 DEGR FT SEC-I **+*** NEW INPUT CARDS **-** REGUIRED 00400 0 1.0 1.8 1.0 1.0 1.0 1.0E-20 00410 0.000 1.44 1.92 1.44 200.0 1.0 1.3 00420 **0 0.0** 0.0 **0.0 0.0** ** EULERIAN REGION INPUT 11005 ' TOPDOWN VIEW OF ROOM COMPARTMENTS ' 1:i000 CARTSN **11** 14 1.0 1.0 10.0 FT 0.0 0.0 11010 NOSLIP NOSLIP NOSLIP NCSLIP NOSLIP NOSLIP 11101 MIXTURE 2 2 8 5 0 14.7 G00.0 600.0 0.9 1.0 0.0 2 2 11102 MIXTURE 2 **6** 4 9 0 14.7 *00.0* 600.0 0.9 1.0 0.0 2 2 11103 MIXTURE 2 10 6 15 0 14.7 600.0 600.0 *0.9* 1.0 **0.0** 2 2 11104 MIXTURE 7 10 8 12 0 14.7 600.0 600.0 **0.9** 1.0 0.0 2 2 11105 MIXTURE **9 10 12 15 0** 14.7 **600.0 600.0 0.9 1.0 0.0** ²**² **** OBSTACLE **CELL** INPUT 11401 NOSLIP 9 2 12 5 1 1 11402 NOSLIP 5 6 12 **9** 1 1 11403 NOSLIP 7 13 8 15 1 1 **** SPECIFIED BOUNDARY INPUT** 11501 INFLOW 2 1 8 1 1'SO1 MIXTURE 14.7 600.0 600.0 0.5 0.0 1.0 11701 0.0 10.0 0.0 10.0 11502 OUTFLOW 13 10 13 15

DATA1: H_2 /WATER BLOWDOWN

FIGURE 4.2: INPUT DATA DECK FOR FIRST SAMPLE PROBLEM

FIGURE 4.3: VELOCITY AND HYDROGEN CONCENTRATION FIELDS AT 0.1 SECOND

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FIGURE 4.4 NELOCITY AND HYDROGEN CONCENTRATION FIELDS AT 0.2 SECOND

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FIGURE 4.5: HYDROGEN CONCENTRATION TRANSIENTS

Long Term Slow Mixing Transient

This problem is based on Test No. 2 of the first phase of Battelle-Frankfurt experiments (see Reference 2 for details). The basic problem and its nodalization are described in Figure 4.6. The simulation spans a real time period of 200 seconds. A **19*C,** 66%/34% (by volume) H_2 / a ir flow is released into the lower central area at a rate of 1.19 m^3 /hr. The initial compartment conditions are assumed to be static air at 17"C. The slow mixing model subcode MITHYD (JSLOW = 1) is utilized for this simulation. A complete input data specification is provided in Figure 4.7.

The hydrogen volume fraction and velocity profile at 20, 100 and 200 seconds into the simulation are plotted in Figures 4.8, 4.9 and 4.10 respectively. The hydrogen concentration transients at five selected locations (see Figure 4.6) are plotted in Figure 4.11. The CPU execution time for this problem is 250 CPU seconds on a CY8ER-176 machine.

Multicompartment Lumped Parameter Model

The third problem is a six region multiconnected geometry defined in Figure 4.12. Hydrogen and air are introduced into the lower central compartment at a rate of $0.32 \text{ m}^3/\text{hr}$. The lumped parameter model with junction characteristics noted in Figure 4.12 is employed. A complete input data deck specification is provided in Figure 4.13. The hydrogen volume fraction transient in the six rooms during the first 10000 seconds of the simulation is reported in Figure 4.14. The 10000 second simulation which utilized a 5 second time step size required less than 60 CPU seconds on a CYBER-176 machine.

FIGURE 4.6 : BASIC 32 NODE MODEL OF BATTELLE FRANKFURT INNER VESSEL USED IN MOST SIMULATIONS

83/10/25. 13.22.25. $-41 -$ PROGRAM DATA2 INPUT FOR SAMPLE PROBLEM 2 ** ' OPEN BF2 SIMULATION - 32 NODES ' 00100 ** BASIC PROBLEM INPUT 00110 0.0 200.0 2.0 SEC 10.0 1 NOXEQ USERDEF 1 1.0E+08 00120 20.0 200.0 00130 AUTODT 100 0.5 1.25 50.0 00140 PRINT NOPRINT PRINT NOPRINT NOPRINT PRINT 00180 2 0 00200 1.0 .000025 .000025 100 1000 0 00220 1 1.0E-50 0.0 0.0 0.0 00230 0 0.0 0.0 1.0E-50 00240 LASL PT LBF/IN2 DEGC M SEC-1 ** NEW INPUT CARDS 00400 0 1.0 1.80 1.0 1.0 1.0 1.0E-20 00410 0.000 1.44 1.92 1.44 200.0 1.0 1.3 00420 00.00.00.00.0 ** EULERIAN REGION DATA 11005 / MESH 1 - LOWER REGION / 11000 AXISYM 6 3 1.0 1.0 0.0 M 0.0 1.0 1 1.216997 1.0 11010 SLIP SLIP SLIP SLIP SLIP SLIP 11020 0.2825 0.2825 0.3092 0.3401 0.3741 0.4115 11030 1.0 1.0 1.0 11050 NOFILM 11101 AIR 2 2 7 4 0 14.7 17.0 17.0 1.0 1.0 0.0 2 2 21005 ' MESH 2 - UPPER REGION ' 21000 AXISYM 7 2 1.0 1.0 0.0 M 0.0 1.0 1 1.216997] 1.0 21010 SLIP SLIP SLIP SLIP SLIP SLIP 21020 0.2825 0.2825 0.3092 0.3401 0.3741 0.4115 0.4501 21030 1.0 0.8138 21050 NOFILM AIR 2 2 8 3 0 14.7 17.0 17.0 1.0 1.0 0.0 2 2 21101 ** HYDROGEN - AIR SOURCE 03010 AIR 1 2 2 03011 0.0 DEGREES 0.0657 1.0 1.0 0.0 2 0.0 03060 AIR 1 3 2 03011 0.0 DEGREES 0.2701 1.0 1.0 0.0 2 0.0 03110 AIR 1 4 2 03011 0.0 DEGREES 0.6642 1.0 1.0 0.0 2 0.0 03011 SEC KG/SEC J/KG M SEC-1 0.0 1.367E-04 2.934E+05 0.0 03012 03013 10000.0 1.367E-04 2.934E+05 0.0 03160 HYD 1 2 2 03161 0.0 DEGREES 0.0657 1.0 1.0 0.0 2 0.0 03210 HYD 1 3 2 03161 0.0 DEGREES 0.2701 1.0 1.0 0.0 2 0.0 03260 HYD 1 4 2 03161 0.0 DEGREES 0.6642 1.0 1.0 0.0 2 0.0 03161 SEC KG/SEC J/KG M SEC-1 03162 0.0 1.828E-05 4.181E+06 0.0 10000.0 1.828E-05 4.181E+06 0.0 03163 ** COUPLING 006001 TOP 1 2 4 2 2 2 2 2

DATA2: BF2 SHORT TERM DATA

FIGURE 4.7: INPUT DATA DECK FOR SECOND SAMPLE PROBLEM

VOLUME FRACTION **112**

FIGURE 4 **8 : BF2** SIMULATION **AT 20 SECONDS**

FIGURE '4.9 : BF2 SIMULATION AT 100 SECONDS

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H₂ VOLUME FRACTION X 1000

FIGURE 4.10: BF2 SIMULATION AT 200 SECONDS

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FIGUPE 4.11: HYDROGEN CONCENTRATION TRANSIENTS

 $\label{eq:2.1} \mathcal{L}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}})) = \mathcal{L}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}})) = \mathcal{L}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}(\mathcal{L}^{\mathcal{L}}_{\mathcal{L}}))$ χ . ~ 100 km s $^{-1}$

FIGURE 4.12 **:** PROBLEM GEOMETRY **AND CONNECTION** LOGIC FOR SIX ROOM **LUMPED** PARAMETER PROBLEM

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dd/10/20. Id.2d.40. PROGRAM **DATA3 - 47 -+*** INPUT FOR **SAMPLE** PROBLEM **3** 00100 ' 6 ROOM LUMPED PROSLEM ' **-;.** BASIC PRO2LEM INPUT 00110 0.0 10000.0 5.0 SEC 10.0 1 NOXEa USERDEF 2 I.OE+06 00120 500.0 10000.0 00130 CONST 100000 **0.5** 1.25 5.0 00140 PRINT NOPRINT NOPRINT NOPRINT NOPRINT PRINT **0)01'0 1 6 5.0** 00200 1.0 0.00010 0.00010 50 20000 0 **00220** 1 0.0 0.0 0.0 0.0 00230 0 0.0 0.0 0.0 (00240 LASL PT LBF/IN2 DEGC M SEC-I **** NEW** INPUT CARDS 00400 0 1.0 1.8 1.0 1.0 1.0 1.OE-20 00410 0.000 1.44 **1.92** 1.44 200.0 1.0 1.3 00420 0 0.0 0,0 0.0 0.0 -* EULERIAN MESH DATA 11005 ' DUUMY MESH - REGUIRED 11000 CARTSN 1 1 1.0 1.0 1.0 M **0.** 1.0 1 1.2212081 **1.0** 11010 SLIP SLIP SLIP SLIP SLIP SLIP **¹¹¹⁰¹**AIR 2 **2** 2 2 0 14.7 16.0 16.0 1.0 1.0 0.0 2 2 ****** LUMPED PROBLEM DATA 12005 ' ROOM **1** ' 12000 ZEROD 40.5 M3 0.0 0.0 0.0 12010 AIR 14.7 16.0 22005 ' ROOM 2 22000 ZEROD 30.2 M3 0.0 0.0 0.0 22010 AIR 14.7 16.0 32005 ' ROOM **5 ' 32000** ZEROD 41.1 **M3 0.0 0.0 0.0** 32010 AIR 14.7 **16.0** 42005 ' ROOM 6 **'** 42000 ZEROD 38.9 M3 0.0 0.0 0.0 42010 AIR 14.7 **16.0** 52005 ' ROOM 7 *'* **52000** ZEROD 40.4 M3 0.0 0.0 0.0 52010 AIR 14.7 **16.0** 62005 ' ROOM 8 62000 ZEROD 38.3 M3 0.0 0.0 0.0 62010 AIR 14.7 16.0 ****** SOURCE ADDITION TO ROOM 1 03010 AIR **i** 0 0 03011 0.0 DEGREES 1.0 1.0 1.0 0.0 2 **O,O** 03011 SEC KG/SEC J/KG M SEC-1 03012 0.0 3.7147E-05 2.90457E+05 0.0 03013 100000.0 3.7147E-05 2.90457E+05 0.0 03060 HYD 1 0 **0** 03061 0.0 DEGREES 1.0 **1.0** 1,0 **010** 2 010 03061 SEC **KG/SEC J/KG** M SEC-1 **03062** 0.0 4.9667E-06 4.13804E+06 0.0 03063 100000.0 4.9667E-06 4.13804E+06 0.0 **-e** COUPLING SPECS o9001 1 1 4 3.8 3.8 **0.60** 0.0 06002 2 4 3 0.20 0.20 0.20 **0.0** 09003 3 3 2 25.5 25.5 0.90 0.0 FIGURE 4.13: INPUT DATA DECK FOR 09004 4 1 **6** 3.8 3.8 0.60 0.0 THIRD SAMPLE PROBLEM **09005 5 6 5** 0.20 **0.20** 0.20 **0.0** THIRD SA **09006 I 5** 2 **12.8** 12.8 0.50 0.0

HYDROGEN VOLUME FRACTION (8)

FIGURE 4.14: ROOM HYDROGEN CONCENTRATION TRANSIENTS

FOR LUMPED PARAMETER PROBLEM

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5.0 Conclusion

This manual addresses the needs of those using the containment hydrogen analysis code, LIMIT, developed at MIT. The format and content assumes the availability of both the users manual of the BEACON code and the report of Manno and Golay. Input formats are specified, job control language are reviewed and sample problems are presented.

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6.0 References

- 1. C.R. Broadus et al., BEACON/Mod 3: A Computer Program for Thermal Hydraulic Analysis of Nuclear Reactor Contaminants - Users Manual, NUREG/CR-1148, April 1980.
- 2. V.P. Manno and M.W. Golay, Analytical Modelling of Hydrogen Transport in Reactor Containments, MIT Energy Laboratory Report, MIT-EL 83-009, September, 1983.
- 3. R.J. Wagner et al., "NRTS Environmental Subroutine Manual," USDOE, 1977.
- 4. NOS Computing Service Reference Set, Volumes 1 to 3, Control Data Corporation, Publication No. 84000320, 1981.
- 5. NOS Computing Service UPDATE 1, Control Data Corporation, Publication No. 84001580, 1981.
- 6. NOS Computing Service CYBER Loader Version 1, Control Data Corporation, Publication No. 84001620, 1980.
- 7. XEDIT Extended Text Editor, Control Data Corporation, Publication No. 76071000, 1980.