VERIFICATION AND VALIDATION OF TMAP4

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ABSTRACT

The Tritium Migration Analysis Program MOD1/CY04 (TMAP4) was written to be used in analyzing experiments and for safety calculations that involve the injection, solution, diffusion, trapping, release, and other related processes experienced by hydrogen isotopes in materials. Because of the desire to make it suitable for analyzing safety issues, it is important that TMAP4 be certified (verified and validated) at Quality Assurance Level A. This report documents the work done to achieve that certification. The process includes assuring that the developed code meets the software requirements specified in the Software Quality Assurance Plan, verifying that the code functions in accordance with the written description and that it is self-consistent and internally correct, and validating that its computed results are in agreement with experimental data and/or known analytical solutions. Quality Level A certification for TMAP4 is specifically for implementation on an IBM PS/2 Model 70 operating under DOS 5.0. Certification for any other environment will require demonstration that all of the verification and validation tests documented here give the same results in the new environment.

CONTENTS

FIGURES

TABLES

INTRODUCTION

The Tritium Migration Analysis Program MOD1/CY04 (TMAP4) was developed by the Fusion Safety Program at the Idaho National Engineering Laboratory by EG&G Idaho, Inc. as a tool for analyzing processes and systems that involve the interaction of tritium or other hydrogen isotopes with structures and enclosures that make up a fusion reactor system. However, it is much more versatile than that. The code accomplishes heat and mass transfer calculations in one-dimensional structures and associated zero-dimensional enclosures. Specific processes encompassed are local heat generation and mass addition (by implantation, for example), diffusion, dissociation and recombination at surfaces, trapping and release from traps in structures, chemical reactions in enclosure volumes, and flows between enclosures and across enclosure-structure interfaces. A detailed description of the code is provided in the TMAP4 User's Manual.[1] There are two parts to the code that are subject to verification and validation. One is the preprocessor that converts the user-written input deck into a form appropriate for analysis, including a compilable FORTRAN subprogram called TAPE7.FOR if equations are used in the input file. The other is the computational module that actually performs the calculations.

To be eligible for use in analyses supporting or serving as a basis for decision involving safety-related systems, structures, components, or services where failure could cause undue risks to employees or to the public health and safety, a computer code must be certified to meet Quality Level A. The process of achieving that certification within EG&G Idaho is specified by Nuclear Engineering Standard Practice NE-SP-1 which delineates the requirements for preparing a Software Quality Assurance Plan. Those requirements are based on industry standards: ANSI/IEEE Standard 730-1984 for Software Quality Assurance Plans, ANSI/IEEE Standard 830-1984 for Software Requirements Specifications, ANSI/IEEE Standard 1012-1986 for Software Verification

and Validation Plans, and ANSI/IEEE Standard 828-1983 for Software Configuration Management Plans.

In summary, a Software Quality Assurance Plan (SQAP) is prepared that delineates requirements for the code itself, the verification and validation process, and configuration control. A number of tests are made on the code to assure that (1) the coding is correct and consistent with the theoretical model on which it is based, (2) the code performs in accordance with the stated characteristics in the code documentation, and (3) the results are consistent with physical observations or known solutions over the range of problems for which the certification is made. Success in reaching those objectives is determined by a Software Quality Assurance Board (SQAB). This report documents that process for TMAP4 operating on an IBM PS/2 Model 70 with DOS 5.0.

Once the code has been verified and validated, it is placed under Software Configuration Control (SCC) procedures which are under the direction of a Software Configuration Control Coordinator (SCCC). The SCCC maintains the permanent record copy and a backup copy of the code and all supporting documentation. Any changes or maintenance done on the code must conform to the requirements set forth in the SQAP and be approved by the SQAB.

The certification is done for a specific operating environment, in this case an IBM PS/2 Model 70 operating under DOS 5.0. Before certification may be granted to an changes or upgrades in the code or to the existing code in a different operating environment, the same process of verification and validation must be undertaken for the changed circumstances. Only when it has been determined that results in the new environment are equivalent to (or better if flaws are found in the original) the original code may the SQAB grant certification for that environment and/or the new configuration.

In what follows we describe in detail the requirements and the work done to satisfy the requirements for verification and validation of TMAP4. The requirements are specified in the Software Quality Assurance Plan for TMAP4, Fusion Safety Program and Fuels and Materials Unit, June 24, 1992. The processes of verification and validation have uncovered several weaknesses in the code. These do not impact the accuracy of calculations, but do suggest improvements for future development iterations.

VERIFICATION

The following is extracted from the SQAP as a definition of the tasks required for verification of TMAP4.

> The verification of the preprocessor stage is required to ensure that all applicable diagnostic error detection and processing of all user entered data performs intended and designed. This verification assessment will use one or more input models to exercise all available input options in TMAP4. It will involve extensive and systematic assessments of error diagnostic detection of each input parameter within the input deck which is composed of several input blocks. The process will impose systematic errors at each applicable parameter position within an input stream. four types of formats will be used for each possible input parameter: 1) a hollerith format, 2) an integer number format, 3) a real (fixed decimal) number format, and 4) an exponential number format. One format will always be the correct format. for each imposed error type, the resulting error message will be assessed to assure a proper "error processed" execution termination, as well as the appropriateness of the diagnostic response(s). For each selected input deck, the results of all four error format types will be documented along with any generated diagnostic error messages related to the imposed error. The documentation will also include the original error-free input deck(s) to allow error re-construction audits.

> To limit the scope of this assessment, several items will be excluded: 1) the "Title Input" block since it only performs title input processing and has no effect on the final quality level of this code, 2) repeated input parameters, such as those encountered in multiple diffusion and thermal segments and multiple table definition inputs since they utilize the same set of error checking statements [Note: Repeated segments and tables will be checked by multiple duplication of already verified segments/tables - up to the allowed limits (see Section 3.4)], and 3) the "Equation Input" block since its error assessments are performed by an external FORTRAN compiler.

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3

The main transient execution stage of the code will be verified in two parts. The first part will utilize several complex models (limited to the ones developed for the preprocessor validation) to show the functionality of all available options and to allow general assessments of the validity of the predicted results (i.e., no flow through "nonflow" boundary conditions, depletion of source concentrations, development of expected diffusion gradients, etc.). These input decks will be documented and described along with a qualitative description of the expected and obtained numerically predicted results.

The second part of the main transient execution stage verification will use preprocessor verified input models to provide a general assessment of the TMAP4 program structure. This process will utilize the Coverage Analysis Tools available at the INEL by the Scientific Computing Unit (#4C20, POC: Earl Marwil or designated alternate) to identify major logic paths, to assess the amount of executable code utilized, to check subroutine utilization efficiencies, etc. The objective of this second stage is to identify (and eliminate if necessary) any unused program coding and to assure that all applicable program structure has been utilized. The documentation of this stage of the verification will again require a description and listing of the chosen input decks and must provide a summary and description of the Coverage Analysis Tools results.

Verification was accomplished in two parts. The first addressed the preprocessor module and was mainly concerned with error detection. The second exercised both the preprocessor and computational module to ensure proper operation and to apply the coverage analysis techniques available. Validation was an exercise to establish the agreement between TMAP4 results and manual analytical solutions for selected problems. We now discuss these in detail.

Preprocessor

Verification of the preprocessor module of TMAP4 is required to ensure that all applicable diagnostic error detection and processing of all user-entered data perform as intended and designed. Systematic assessments of the TMAP4 input options have been performed through a process which imposes specified errors at each applicable parameter location within a given input parameter stream. For each imposed error type,

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the resulting error message was assessed to assure proper error processing, appropriateness of the error response, and execution termination.

Verification of the preprocessor included an error assessment of seven of the nine input blocks. Those included were:

1.   Main Input
1.   Enclosure Input
2.   Thermal Segment Input
3.   Diffusion Segment Input
6.   Table Input
5.   Control Input
7.   Plot Input

The Title Input block was ignored since it has no computational effect on the execution of the code. The Equation Input block was also omitted since error assessments are handled externally by the FORTRAN compiler. Assessment of the code's input limits as stated in Section 3.4 of the SQAP is implicit in this analysis.

Two approaches were utilized in imposing specified errors at each parameter location based upon whether the input parameter required single parameter inputs (may or may not be repeating) or multiple data values. A single parameter input is illustrated as follows:

```
DSPCNME = t1,t2,t3,end[repeating single input parameter]
          ↑
          Primary input parameter
```

In this case, the primary input parameter is varied between a real, and integer, an hollerith, or an exponential format. Only one parameter is varied as the resulting error message is common to all of them.

A multiple data input parameter differs from the single input as shown in the following example:

```
               Secondary Input Parameter
                           ↓
    HTRBCL = CONVEC,const,1.5,ENCL,1,end
                        ↑
         Primary Input Parameter
```

The primary input may take the form of a repeating data value, a constant qualifier with
a single data value (as shown above), or an equation or table identifier with a single data
value, while the secondary input is typically a single parameter of a specified format.
For this type of input stream, only the primary input parameter was formally assessed.
The secondary input was varied from its specified format to assure proper error
detection and termination, but formal presentation of this data is not presented. The
results for the input blocks listed previously are presented in Tables 1 through 6. Results
for Table Input are not presented in tabular form because this section was only checked
for consistency with the stated format in the manual. This input block was found to
behave as stated in the TMAP4 User's Manual.

TABLE 1 MAIN INPUT ANALYSIS

Main	Real	Integer	Hollerith	Exponential
DSPCNME	▢	▢	✓	▢
ESPCNME	▢	▢	✓	▢
SEGNDS	⊠[1]	✓	⊠[1]	⊠[1]
NBRENCL	⊠[2]	✓	⊠[2]	⊠[2]
LINKSEGS	⊠[3]	✓	⊠[3]	⊠[3]

Key: ✓Results are as expected
          ⊠Error message received; see # below for error message.
          ▢Alphabetic format is indicated in manual - no message returned.

Error Messages:

          1"...nbr. of seg. nodes at word -2- is not an integer value."
          2"...integer value expected after +nbrencl+."
          3"...integer segment nbr. expected."

6

TABLE 2 ENCLOSURE INPUT ANALYSIS

Enclosure	Const				Equ				Tabl				Comments
	R	I	H	E	R	I	H	E	R	I	H	E	
ETEMP	✓	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	⊠[2]	Only real numbers are allowed
ESPPRES													
FUNC	✓	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	Func → value(r)
BDRY	✓	⊠[6]	⊠[6]	⊠[6]	⊠[7]	✓	⊠[7]	⊠[7]	⊠[8]	✓	⊠[8]	⊠[8]	Bdry → value(r),Const,Equ,Tabl
REACTION	✓	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	⊠[4]	Does not apply to Bdry enclosure
EVOL	✓	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	⊠[5]	Only real numbers are allowed
OUTFLOW	⊠[1]	⊠[1]	□	□	✓	□	□	□	✓	□	□	□	Function of time only

Key:
R = Real
I = Integer
H = Hollerith
E = Exponential

✓ Results are as expected
⊠ Error message received; see # below for error message. Execution with this parameter type is suspect
□ Error message expected but none returned.

Error Messages:

1 "...+qflow+ must be a const, equ, or tabl."
2 "...expecting floating pt. encl. temperature."
3 "...only real valued initial pressures are allowed for +func+ encl."
4 "...expecting real number after enclosure species."
5 "...real nbr. expected for enclosure volume"
6 "...no floating point nbr found as data."
7 "...eqn integer...format violated."
8 "...tabl, integer...format violated."

7

TABLE 3 THERMAL SEGMENT ANALYSIS

Thermal	Repeat				Const				Equ				Tabl				Comments
	R	I	H	E	R	I	H	E	R	I	H	E	R	I	H	E	
DELX	✓	⊠2	⊠4	✓	□	⊠5	⊠5	□	⊠4	⊠4	⊠4	⊠4	⊠4	⊠4	⊠4	⊠4	Valid inputs are reals and constants
DTEMP	✓	⊠2	⊠2	✓	✓	⊠5	⊠5	✓	⊠4	⊠4	⊠4	⊠4	⊠4	⊠4	⊠4	⊠4	Valid inputs are reals and constants
TCON	□	⊠3	⊠3	□	✓	⊠3	⊠3	✓	⊠6	✓	⊠6	⊠6	⊠7	✓	⊠7	⊠7	Function of T and/or t only
RHOCP	□	⊠3	⊠3	□	✓	⊠3	⊠3	✓	⊠6	✓	⊠6	⊠6	⊠7	✓	⊠7	⊠7	Function of T and/or t only
HSRC	□	⊠3	⊠3	□	✓	⊠3	⊠3	✓	⊠6	✓	⊠6	⊠6	⊠7	✓	⊠7	⊠7	Function of x and/or t only
HTRBCL/R																	Applies to surfaces only
ADIAB	□	□	□	□	□	□	□	□	□	□	□	□	□	□	□	□	No data required
CONVEC	⊠1	⊠1	⊠1	⊠1	✓	□	□	✓	✓	✓	□	□	□	✓	□	□	
STEMP	⊠1	⊠1	⊠1	⊠1	✓	□	□	✓	✓	✓	□	□	□	✓	□	□	
SFLUX	⊠1	⊠1	⊠1	⊠1	✓	□	□	✓	✓	✓	□	□	□	✓	□	□	
LINK	⊠9	⊠9	⊠9	⊠9	✓	⊠9	⊠9	⊠9	⊠9	⊠9	⊠9	⊠9	⊠9	⊠9	⊠9	⊠9	No data required
HGAP	⊠8	⊠8	⊠8	⊠8	✓	□	□	✓	□	✓	□	□	□	✓	□	□	Only used with linked segments

Key: R = Real
      I = Integer
      H = Hollerith
      E = Exponential

✓ Results are as expected
⊠ Error message received; see # below for error message.
□ Error message expected but none returned. Execution with this parameter type is suspect

Error Messages:

1   "illegal format for boundary condition"
2   "no int. or floating pt. nbr found as data"
3   "no floating pt. nbr found as data"
4   "only real or constant format allowed"
5   "no floating pt. data found"
6   "...equ, integer,...format violated"
7   "...tabl, integer,...format violated"
8   "...illegal format for +hgap+ input"
9   "no +end+ statement found on boundary condition type"

8

TABLE 4 DIFFUSION SEGMENT ANALYSIS

Diffusion	Repeat				Const				Equ				Tabl				Comments
	R	I	H	E	R	I	H	E	R	I	H	E	R	I	H	E	
DCONC	✓	⊠[4]	⊠[4]	✓	⊠[4]	⊠[4]	✓	✓	⊠[5]	✓	⊠[5]	⊠[5]	⊠[6]	✓	⊠[6]	⊠[6]	Valid inputs are reals and constants
DCOEF	☐	⊠[4]	⊠[4]	☐	✓	⊠[4]	⊠[4]	✓	⊠[5]	✓	⊠[5]	⊠[5]	⊠[6]	✓	⊠[6]	⊠[6]	Function of T and/or t only
QSTRDR	☐	⊠[4]	⊠[4]	☐	✓	⊠[4]	✓	✓	⊠[5]	✓	⊠[5]	⊠[5]	⊠[6]	✓	⊠[6]	⊠[6]	Function of T and/or t only
SPCSRC	☐	⊠[4]	⊠[4]	☐	☐	⊠[4]	✓	✓	⊠[5]	✓	⊠[5]	⊠[5]	⊠[6]	✓	⊠[6]	⊠[6]	Function of t and/or x only
DIFBCL/R																	Applies to surfaces only
RATEDEP	⊠[7]	⊠[7]	⊠[7]	⊠[7]	✓	☐	✓	✓	☐	✓	☐	☐	☐	✓	☐	☐	Tabl. → f(T), Equ. → f(t,T)
LAWDEP	⊠[1]	⊠[1]	⊠[1]	⊠[1]	☐	☐	✓	✓	☐	✓	☐	☐	☐	✓	☐	☐	
SCONC	⊠[2]	⊠[2]	⊠[2]	⊠[2]	☐	☐	✓	✓	☐	✓	☐	☐	☐	✓	☐	☐	Function of T and/or t only
NONFLOW	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	⊠[8]	No data required
LINK	⊠[1]	⊠[1]	⊠[1]	⊠[1]	✓	☐	✓	✓	☐	✓	☐	☐	☐	✓	☐	☐	
SURFA	✓	⊠[3]	⊠[3]	✓	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	⊠[3]	Valid inputs are reals and exponentials

Key:

R = Real
I = Integer
H = Hollerith
E = Exponential

✓ Results are as expected
⊠ Error message received; see # below for error message. Execution with this parameter type is suspect
☐ Error message expected but none returned
• Non-repeating values were used

Error Messages:

1. "+solcon+ must = const, tabl, or equ"
2. "the +sconc+ b.c. must = const, tabl, or equ"
3. "floating pt. nbr expected after +surfa+"
4. "no floating pt. nbr found as data"
5. "...equ, integer,...format violated"
6. "...tabl, integer,...format violated"
7. "+ksubd/r+ must = const, equ, or tabl"
8. "+end+ does not follow +nonflow+ on card"

TABLE 5 CONTROL INPUT ANALYSIS

Main	Real	Integer	Hollerith	Exponential
TIME	✓	□	□	✓
TSTEP	✓	□	□	✓
TIMEND	✓	□	□	✓
NPRINT	□	✓	□	□
ITERMX	□	✓	□	□
DELCMX	✓	□	□	✓

Key: ✓   Results are as expected

            □   Error message expected but none returned. Execution with this parameter type is therefore suspect.

TABLE 6 PLOT INPUT ANALYSIS

Main	Real	Integer	Hollerith	Exponential
NPLOT	□	✓	□	□
PLOTSEG	□	✓	⊠[1]	□
PLOTENCL	□	✓	⊠[2]	□
DNAME	☺	☺	☺	☺
ENAME	☺	☺	☺	☺
DPLOT	✓	✓	✓	✓
EPLOT	✓	✓	✓	✓

Key: ✓   Results are as expected

            ⊠   Error message received; see # below for error message.

            □   Error message expected but none returned. Execution with this parameter type is therefore suspect.

            ☺   Alphabetic input specified. Execution will proceed if D/ESPCNME and D/EPLOT are consistent.

Error Messages:

1   "...expecting integer for diffusion segment."

2   "...expecting integer for enclosure number."

Additional input restrictions observed were that a "reaction array out-of-bounds" error will result when greater than 20 reactions are attempted. Also, it was confirmed that the "end" statement must immediately follow a delimiter such as a comma or a carriage return. It may not appear on a line by itself unless it begins in column 1.

There were numerous instances in the tables preceding where error messages were expected for a given data type, but none were returned. Execution of the code with these erroneous inputs needs to be performed to assess the effect these parameters impose. Additionally, error checking routines will need to be included or modified to flag these invalid data parameters. Both issues will be addressed in the next code revision and release. Correct input data type results in correct results, and we have elected not to make changes suggested by □ in the tables at this time.

Computational Module Analysis

The following analysis was provided by the Scientific Computing Unit of EG&G Idaho, Inc. It represents an independent assessment of the quality of the code from the perspective of specialists in scientific computing who were not previously acquainted with it. Some specific comments they present will be replied to in following sections.

> The TMAP4 program consists of a preprocessor program, TMAPP4, and a computational processor, TMAPC4. Thirty-seven sample problems were supplied along with the source code. All files were uploaded from a Macintosh PC to the INEL Cray X/MP-216 for assessment and analysis. Each program was analyzed using the CRAFT (Cross Reference Analysis of FORTRAN) tool, FORWARN, the FORTRAN 77 analyzer, and PC-Metric. These tools provide static analysis, coverage analysis, and complexity analysis.

Functions

TMAPP4 contains one function, *nextcrd*, with an alternate entry point, *inciv.*. One function, *wrtcrd*, is not called by any routine in TMAPP4.[a]

There were no alternate entry points in TMAPC4 and no unreferenced functions.

Common Block Irregularities

The common blocks used in both codes are generally consistent. A checkpoint and restart capability of the code uses equivalencing as a technique to write and read data from and to certain common blocks. This technique contributes to making the code less readable and more difficult to trace the use of variables used in those common blocks. The equivalence of a local array name (of length 1) to an array in common (of length greater than 1) generates a warning message. The arrays should be of the same size to avoid potentially introducing defects during code maintenance..

In the program TMAPP4, the following definition irregularities were observed: The array *cardc* in common block *card2* is undefined and used. The variable *iblank* in common block *cmn0* is defined but unused. The variable *nra* in common block *cmn0a* is defined but unused. There are a number of instances where a common block is declared in a module but none of its elements are used or modified. These could be removed from the code to reduce clutter and improve readability.

Since data from TMAPP4 is written to disk and read by program TMAPC4, some of the following require additional analysis to determine whether they contribute to program clutter or are related to the equivalencyg techniques cited above. The arrays *idseg* and *ithrm* in common block *connect* are apparently defined but unused. The array *iqdot* in common block *instr* is also apparently defined but unused. Variables and arrays *icouple, ncyc, itermx, nprint, nloop, itera, nplotd, nplote,named, namee,* and *iplot* in common block *integ* are apparently defined but unused. Arrays and variables *asurf, srcse,*

---

[a] The alternate entry point is accessed while reading and processing the data statements in the input deck and is particularly useful when an input statement extends beyond one line. The subroutine *wrtcrd*, was included as a means of conveniently displaying the values read and processed by the preprocessor. It is a utility for code improvement and maintenance and should not be accessed during user operation of the code. It could be removed with no consequence to code performance, but is retained for future convenience.

12

vole, qdot, cetrpi, and *dennum* in common block *names* are apparently defined but unused.

In TMAPC4 there are a number of entities in common with potential definition irregularities (undefined and unused, defined and unused, or used but undefined). Further analysis would be necessary to determine whether these are defined when reading the binary input data file generated by TMAPP4. There are a number of instances where a common block is declared in a module but none of its elements are used or modified. These could be removed from the code to reduce clutter and improve readability.

In some blocks, an implicit equivalence of two variable names sharing the same memory location occurs where the names differ by one character and one variable name is used in only one module. These include: *icbe* and *ipbe* in block *instr, ncbe* and *npbe* in *instr,* and *itera* and *iterct* in block *integ.*

Interface Irregularities

In both TMAPP4 and TMAPC4 there are local variables which are apparently defined but unused. A further inspection is required to determine if these are actually used or whether they contribute to program clutter.

In addition, in TMAPP4 routines *dimchk, instr2, instr3,* and *relnbr* have an argument which is a fixed length character variable. The calling routines use a character constant. This situation frequently results in a length conflict between the character constant and the character variable. (Most compilers simply truncate or pad the constant to the appropriate length.) An easy change to avoid this problem is to declare the character variable to have variable length in the called routines.

FORTRAN Extensions

FORTRAN 77 requires that entity names be no longer than 6 characters. Some entity names in TMAPP4 and TMAPC4 are 7 characters long. This is an extension to the language which is recognized by most compilers. FORTRAN 90 allows up to 31 characters in a name. With the need for more meaningful naming conventions, long entity names should not be shortened to conform to the standard.

The TMAPP4 and TMAPC4 programs are written using lower case characters. This is an extension to the FORTRAN 77 standard.

There is extensive use of the REAL*8 and INTEGER*4 type declarations. The use of the integer constant in this context is nonstandard.

13

In several places a character array element is replaced by a substring of the same element concatenated with another character variable. This is nonstandard due to the potential overlap in a character assignment statement.

Coverage Analysis

Thirty-seven sample problems were supplied. A coverage analysis shows that these problems yield an 80% segment coverage of TMAPP4 and an 87% segment coverage of TMAPC4. Tables 7 and 8 show the percent coverage for each routine.

Complexity Analysis

The complexity measures for both codes indicate very few block IF's and many unconditional GO TO statements. The code was probably developed after the FORTRAN 77 standard was established, but using a style more suited to FORTRAN 66. In addition, the codes have a good ratio of non-blank comments to source code.

Some key metrics are McCabe's cyclomatic complexity, the number of lines of source code, a density of McCabe's cyclomatic complexity per 100 lines of source code, and the number of unconditional GO TO statements. Generally, the routines with the highest complexity are those most likely to have defects. A software maintenance program should focus on those routines with the highest measures.

Details of the complexity analysis appear in Tables 9 and 10 for TMAPP4 and TMAPC4, respectively.

Developer Comments

A careful review of the "defined but not used" and "used but not defined" diagnostics revealed that with three exceptions, all of the variables listed in the above report are appropriately defined and used. *Prima facie* eivdence for that being the case is that the code executes and gives good results. That would not happen if variables were used without being defined. They are defined in TMAPP4 by "data" statements or read in from the "tmapinp" file and passed to TMAPC4 through the "tape1" file where they are restored to the common blocks for use. Exceptions are the variable names

14

cardc, iblank, and *nra* which are defined in TMAPP4 but appear in no other context. Hence, they appear to be excess baggage that could be removed.

TABLE 7 COVERAGE ANALYSIS OF TMAPP4

```
             0        0.20        0.40        0.60        0.80        1.00
             ----+----|----+----|----+----|----+----|----+----|----+----|
BANNER       *********************************************************
CARDCV       ***************************       |           |
CARDRD       *********************************************
CONTROL      *********************************************
DIFF         *************************************************
DIFFBC       ***********************************************
DIMCHK       *****************************************************************
ENCLOSE      *************************************************      |
ERRCHK       ***********************************************************
ERRCVRY      *********************       |           |
FLOW         ********************************       |
GENFLOW      *********************************************
GENREAC      ***********************************************
HSOURCE      ***********************************************
INCIW        ***************************************************************
INSTR2       *******************************************
INSTR3       *********************************************
LOAD         *************************************************
LOX          *********************************************************
MAINP        ***********************************************
PLOT         *****************************************************
REACTIN      ******************************************    |
READE        *************************************************
READRS       *******************************************************************
READT        *****************************************
REFORM       *************************************************
RELNBR       ***************************************************************
SPECDEP      *********************************************************
SPECPFS      *******************************************************
STORE        *************************************************
THERM        *********************************************
THERMBC      *********************************************
TITLE        ***************************************************
TMAPP4       *********************************************************
TRAPIN       *******************************       |           |
WRTBLKS      ***************************************************************
WRTCRD       |    |           |           |           |           |
             ----+----|----+----|----+----|----+----|----+----|----+----|
```
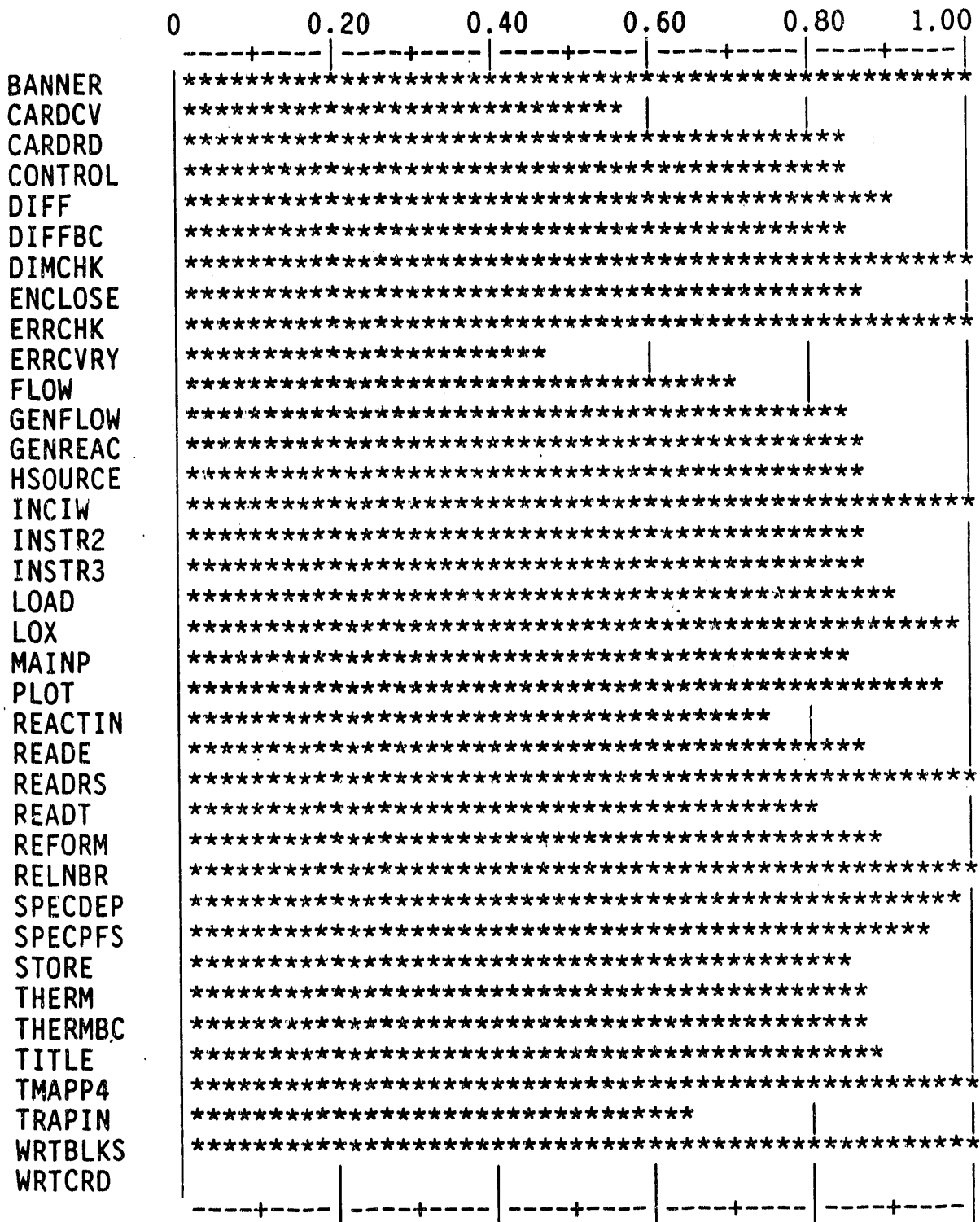
```
      coverage = 0        WRTCRD

0.40 <= coverage < 0.60 CARDCV      ERRCVRY

0.60 <= coverage < 0.80 FLOW        REACTIN     TRAPIN

0.80 <= coverage < 0.85 CARDRD      CONTROL     DIFFBC      GENFLOW
                        MAINP       READT       STORE

0.85 <= coverage < 0.90 ENCLOSE     GENREAC     HSOURCE     INSTR2
                        INSTR3      READE       REFORM      THERM
                        THERMBC     TITLE

0.90 <= coverage < 0.95 DIFF        LOAD        SPECPFS

0.95 <= coverage < 1.00 PLOT        SPECDEP

      coverage = 1.00   BANNER      DIMCHK      ERRCHK      INCIW
                        LOX         READRS      RELNBR
                        TMAPP4      WRTBLKS

   Cumulative coverage = 0.80
```

TABLE 8 TMAPC4 COVERAGE ANALYSIS

```
                  0.20        0.40        0.60        0.80       1.00
          ----+----|----+----|----+----|----+----|----+----
D1DEG1    |********************************
DIFFUSE   |*******************************************************
ENCLOSE   |**************************************************
INCWRD    |****************************************************************
ITER      |*********************************************************
OUTPUT    |***************************************************************
PLOT      |***********************************************************
READBLK   |**************************************************************
SIMQ      |**************************************************
TABLKP    |***************************************************************
THERM     |*************************************
TMAPC     |**************************************************************
TRIDAG    |***********************************************************
UPDSHRC   |***********
UPDMDCO   |*********************************************************
UPDPRES   |*********************************************************
UPDQDOT   |**********************************************
UPDQSTR   |*********************************************
UPDRHCP   |*****************************************
UPDSSRC   |**************************************************************
UPDTCON   |**************************************
UPDTRPR   |*********************************************
UPDTRPT   |**********************************************
          ----+----|----+----|----+----|----+----|----+----|
```

18
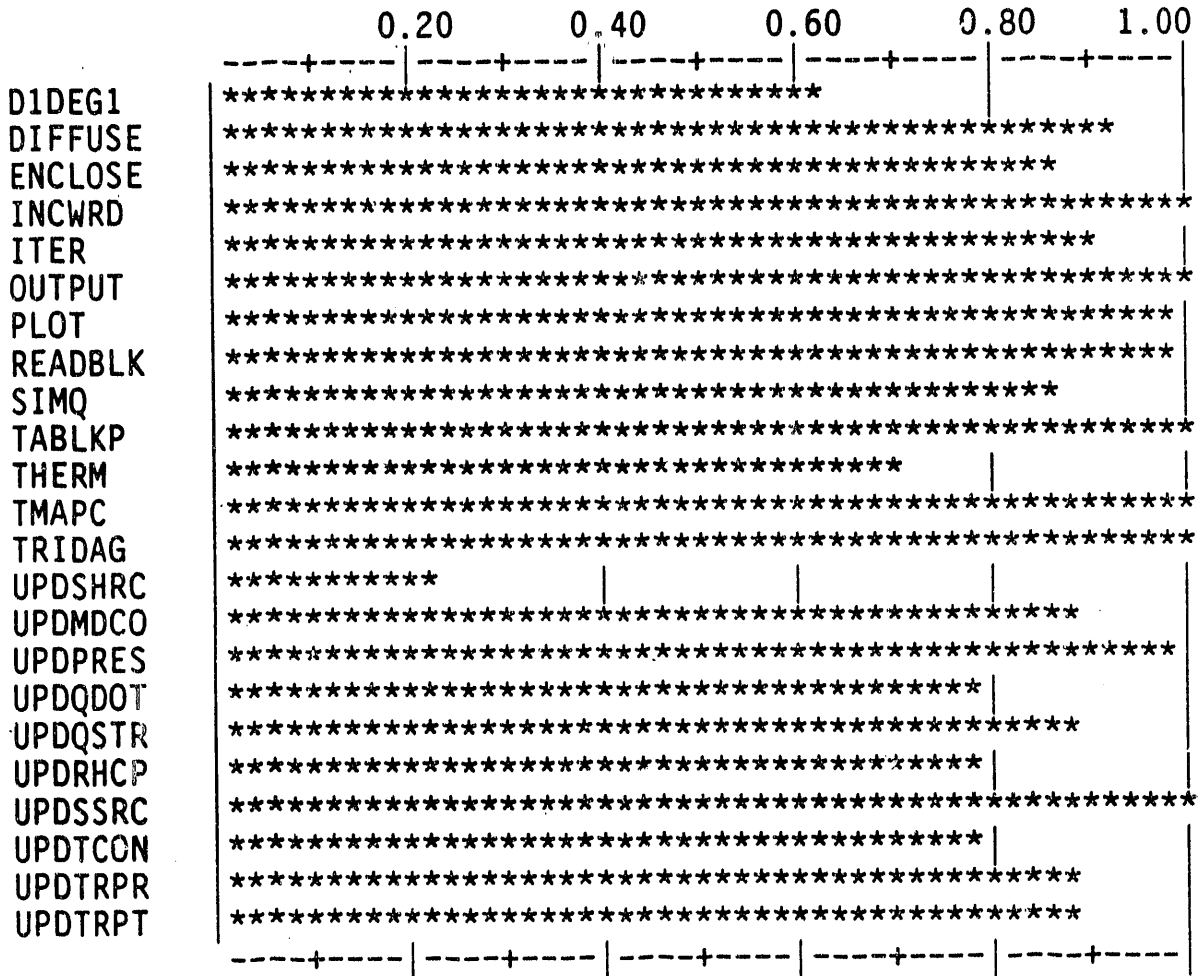
```
0.20 <= coverage < 0.40 UPDHSRC

0.60 <= coverage < 0.80 D1DEG1      THERM       UPDQDOT     UPDRHCP
                        UPDTCON

0.85 <= coverage < 0.90 ENCLOSE     SIMQ        UPDMDCO     UPDQSTR
                        UPDTRPR     UPDTRPT

0.90 <= coverage < 0.95 DIFFUSE     ITER

0.95 <= coverage < 1.00 PLOT        READBLK

        coverage = 1.00 INCWRD      OUTPUT      TABLKP      TMAPC
                        TRIDAG      UPDPRES     UPDSSRC

    Cumulative coverage = 0.087
```

TABLE 9   COMPLEXITY REPORT BY SUBPROGRAM FOR TMAPP4

Name	McCabe's vg1	vg2	loc	den	Bhat	cgoto	ugoto	bIF	lIF	ncomt	rce	Boehm 0.75 months	days	Boehm 1.00 months	days
TMAPP4	4	4	73	6	0	2	0	0	3	32	124	0.15	3.4	0.20	4.5
BANNER	1	1	112	1	0	0	0	0	0	10	40	0.24	5.3	0.32	7.1
CARDCV	109	132	468	29	6	8	100	0	89	78	20	1.08	23.8	1.44	31.7
CARDRD	2	2	60	4	0	0	1	0	1	10	125	0.13	2.8	0.17	3.7
CONTROL	12	13	153	9	1	1	15	5	7	10	17	0.33	7.4	0.45	9.8
DIFF	40	41	396	11	3	1	35	0	22	57	29	0.91	20.0	1.21	26.6
DIFFBC	73	80	769	11	7	1	117	0	66	138	30	1.82	40.1	2.43	53.4
DIMCHK	2	2	23	9	0	0	0	0	1	9	150	0.05	1.0	0.6	1.3
ENCLOS	35	41	287	15	2	1	32	0	27	25	16	0.65	14.2	0.86	19.0
ERRCHK	3	3	52	6	0	0	1	0	2	7	35	0.11	2.4	0.14	3.2
ERRCVRY	10	13	107	13	0	0	9	0	7	25	63	0.23	5.1	0.31	6.7
FLOW	17	19	183	11	1	0	24	0	15	26	29	0.40	8.9	0.54	11.8
GENFLOW	8	8	66	13	0	0	4	0	4	12	35	0.14	3.0	0.18	4.1
GENREAC	6	6	50	12	0	0	2	0	2	10	44	0.10	2.3	0.14	3.0
HSOURCE	6	6	113	6	0	0	4	0	40	22	74	0.24	5.4	0.32	7.1
INCIW	2	2	27	8	0	0	0	0	1	6	75	0.05	1.2	0.07	1.6
INSTR2	9	14	87	17	1	0	9	0	7	34	90	0.18	4.1	0.25	5.4
INSTR3	9	14	89	16	1	0	9	0	7	35	88	0.19	4.2	0.25	5.6
LOAD	12	13	100	13	1	0	15	0	9	19	33	0.21	4.7	0.29	6.3
LOX	3	3	26	12	0	0	0	0	1	10	100	0.05	1.1	0.07	1.5
MAINP	35	39	291	14	2	1	48	0	29	26	16	0.66	14.4	0.88	19.3
PLOT	37	42	270	16	2	3	44	0	24	25	15	0.61	13.4	0.81	17.8
REACTIN	19	23	214	11	1	0	28	0	15	22	20	0.48	10.5	0.63	13.9
READE	23	23	165	14	1	0	15	0	20	18	18	0.36	8.0	0.48	10.6
READRST	2	2	117	2	0	0	1	0	1	10	44	0.25	5.5	0.34	7.4
READT	9	11	92	12	0	0	14	0	8	10	21	0.20	4.3	0.26	5.7
REFORM	15	23	102	23	1	0	16	0	11	25	41	0.22	4.8	0.29	6.4
RELNBR	6	6	44	14	0	0	1	0	4	20	125	0.09	2.0	0.12	2.6
SPCEDEP	12	12	134	9	1	0	17	0	11	24	40	0.29	6.4	0.39	8.5
SPECPFS	17	18	152	12	1	0	9	0	10	27	43	0.33	7.3	0.44	9.7
STORE	30	34	245	14	1	0	35	0	29	70	52	0.55	12.1	0.73	16.1
THERM	27	30	294	11	2	1	34	2	20	29	20	0.66	14.6	0.88	19.5
THRMBC	19	21	167	13	1	1	24	0	16	21	35	0.37	8.1	0.49	10.8
TITLE	6	6	76	8	0	0	7	0	5	8	26	0.16	305	0.21	4.7
TRAPIN	12	12	177	7	1	0	16	0	11	30	43	0.39	8.6	0.52	11.4
WRTBLKS	3	3	166	2	1	0	0	0	0	13	32	0.36	8.0	0.49	10.7
WRTCRD	4	4	41	10	0	0	4	0	1	8	62	0.08	1.8	0.11	2.5

TABLE 10 COMPLEXITY REPORT BY SUBPROGRAM FOR TMAPC4

Name	McCabe's vg1	vg2	loc	den	Bhat	cgoto	ugoto	bIF	lIF	ncomt	rce	Boehm months	0.75 days	Boehm months	1.00 days
TMAPC	7	8	172	5	1	0	4	0	5	38	60	0.38	8.3	0.50	11.1
DIDEGI	8	8	54	15	0	0	6	0	5	15	47	0.11	2.5	0.15	3.3
DIFFUSE	81	83	673	13	11	5	66	0	46	55	12	1.58	34.8	2.11	46.5
ENCLOSE	47	50	273	19	3	0	18	0	27	13	7	0.61	13.5	0.82	18.0
INCWRD	1	1	14	8	0	0	0	0	0	5	125	0.03	0.6	0.04	0.8
ITER	28	32	104	31	1	0	9	0	21	7	8	0.22	4.9	0.30	6.5
OUTPUT	16	16	214	8	2	1	8	0	6	16	16	0.48	10.5	.063	13.9
PLOT	20	35	200	18	2	0	12	0	12	35	33	0.44	9.7	0.59	13.0
READBLK	16	16	163	10	2	0	7	0	10	10	13	0.36	7.9	0.48	10.5
SIMQ	13	13	92	15	1	0	2	0	2	17	29	0.20	4.3	0.26	5.7
TABLKP	1	1	52	2	0	0	0	0	0	6	150	0.11	2.4	0.14	3.2
THERM	25	27	272	10	3	2	39	0	18	20	17	0.61	13.5	0.82	17.9
TRIDAG	3	3	24	13	0	0	0	0	0	4	37	0.05	1.1	0.06	1.4
UPDHSRC	4	4	68	6	0	0	2	0	2	6	43	0.14	3.1	0.19	4.2
UPDMDCO	4	4	70	6	0	0	2	0	2	6	38	0.15	3.2	0.20	4.3
UPDPRES	4	4	69	6	0	0	3	0	3	6	40	0.14	3.2	0.19	4.2
UPDQDOT	4	4	70	6	0	0	2	0	2	6	43	0.15	3.2	0.20	4.3
UPDQSTR	4	4	70	6	0	0	2	0	2	6	38	0.15	3.2	0.20	4.3
UPDRHCP	4	4	70	6	0	0	2	0	2	6	38	0.15	3.2	0.20	4.3
UPDSSRC	4	4	70	6	0	0	2	0	2	6	43	0.14	3.1	0.19	4.2
UPDTCON	4	4	68	6	0	0	2	0	2	6	38	0.15	3.2	0.20	4.3
UPTTRPR	4	4	71	6	0	6	2	0	2	6	38	0.15	3.3	0.20	4.4
UPDTRPT	4	4	70	6	0	0	2	0	2	6	38	0.15	3.2	0.20	4.3

Legend of Metrics in Report

vg1 -- McCabe's cyclomatic complexity metric
vg2 -- McCabe's cyclomatic complexity metric extended
loc -- lines of code
den -- number of decisions per 100 lines of code (vg2/loc)
Bhat -- Halstead's predicted number of errors in writing code
cgoto -- number of COMPUTED GO TO statements
bIF -- number of BLOCK IF statements
lIF -- number of LOGICAL IF statements
ncomt -- number of non-blank comment statements
rce -- number of non-blank comments per 100 executable statements
Boehm 0.75 -- Boehm's estimated time to re-do 75 percent of code
Boehm 1.00 -- Boehm's estimated time to re-do 100 percent of code

21

VALIDATION

The validation assessment of the TMAP4 code is presented in this section. It was done in two parts as outlined in the SQAP. First, comparisons of selected numerical models to analytical solutions were generated. Then comparisons with three sets of experimental results were made. The validation assessment includes descriptions of the input deck along with a copy of the deck on the supplementary disk. Output files are also provided on the supplementary disk, and a comparison is provided here of the calculated results with both theoretical and experimental results.

Comparison with Analytic Solutions

The specific problems to be examined under this phase of validation are listed in the TMAP4 SQAP. The SQAP identified eight such problems for comparison. Filenames for the input files used in these problems are given in parentheses after the problem subheading.

1a) Depleting Source Problem[2] (val-1a.inp)

This model consists of an enclosure containing a finite concentration of atoms which are allowed to diffuse into a SiC layer over time. No solubility or trapping effects are included. The fractional release from the outside of the shell in a depleting source model in a slab geometry is given by:

$$FR = 1 - \sum_{n=1}^{\infty} \frac{2L \sec \alpha_n \exp\left(-\alpha_n^2 \frac{DT}{l^2}\right)}{L(L + 1) + \alpha_n^2} \tag{1}$$

where

$$L = \frac{lA}{V\phi}$$

$$\phi = \frac{\text{source concentration}}{\text{layer concentration}}$$

where the layer concentration is that at the interface with the source (ϕ is constant in time),

A = surface area

V = source volume

l = layer thickness

and the α_n are the roots of

$$\alpha_n = \frac{L}{\tan \alpha_n}$$

The results of TMAP4's calculated release are shown in Table 11 along with the analytical solution. Column 4 of the table presents the variation of TMAP4's calculated results on the IBM PS 2/70˙ compared with the analytical solution expressed as:

$$\text{Variation} = \frac{\text{TMAP4˙Value} - \text{Analytical Value}}{\text{Analytical value}}$$

Except for the early times (i.e., 0 - 10 seconds), agreement between TMAP4 and the analytical solution are generally within 1% with TMAP4 overpredicting the fractional release. At later times, TMAP4 slightly underpredicts. The analytical solution was obtained by discarding series terms with a contribution of less than 1.0E-10 using Lotus 123™ release 3.0 on and IBM PS 2/70. Table 11 presents the initial 45 seconds of a 140 second analysis. Beyond 45 seconds, the variation between the two results remains less than 1%. Figure 1 shows the comparison in graphic format.

TABLE 11 COMPARISON OF TMAP4 AND ANALYTICAL RESULTS FOR A DEPLETING SOURCE PROBLEM

Time (s)	TMAP4	Theory	Variation
0	0	0	0
1	0.000644	6.0E-07	1081.268
2	0.002831	0.000262	9.806189
3	0.007223	0.002399	2.010316
4	0.014077	0.007873	0.7881
5	0.023316	0.016781	0.389429
6	0.034657	0.028554	0.213738
7	0.047736	0.042499	0.12323
8	0.058001	0.06218	0.072051
9	0.077649	0.074568	0.041318
10	0.093853	0.091823	0.022112
11	0.110548	0.109482	0.009737
12	0.127545	0.127337	0.001637
13	0.144693	0.145233	-0.00372
14	0.161873	0.163059	-0.00727
15	0.17899	0.180733	-0.00964
16	0.195987	0.198197	-0.01115
17	0.212795	0.21541	-0.01214
18	0.22939	0.232343	-0.01271
19	0.245738	0.248977	-0.01301
20	0.261816	0.265301	-0.01314
21	0.27761	0.281307	-0.01314
22	0.293121	0.296991	-0.01303
23	0.30833	0.312353	-0.01288
24	0.323243	0.327395	-0.01268
25	0.337859	0.342119	-0.01245
26	0.352174	0.356529	-0.01222
27	0.366192	0.37063	-0.01197
28	0.379914	0.384426	-0.01173
29	0.393354	0.397923	-0.01148
30	0.406503	0.411126	-0.01125
31	0.419375	0.424042	-0.01101
32	0.43197	0.436677	-0.01078
33	0.444295	0.449035	-0.01056
34	0.456355	0.461122	-0.01034
35	0.46815	0.472945	-0.01014
36	0.4797	0.484509	-0.00993
37	0.490991	0.49582	-0.00974
38	0.502044	0.506883	-0.00955
39	0.512857	0.517703	-0.00936
40	0.52343	0.528286	-0.00919
41	0.533777	0.538637	-0.00902
42	0.543904	0.54876	-0.00885
43	0.55381	0.558662	-0.00869
44	0.563495	0.568346	-0.00854
45	0.572973	0.577818	-0.00838

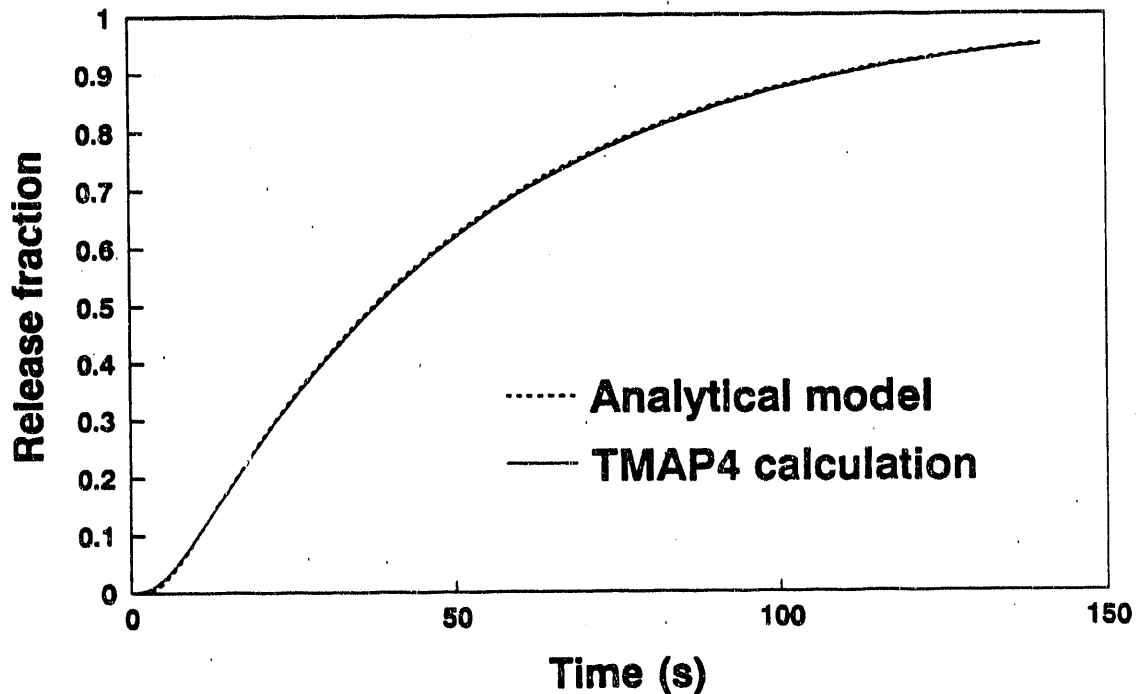# Depleting Source Problem
SQAP Reference 4.2.1.a

Figure 1. TMAP4 gives excellent results in comparison with the analytical solution for the depleting source problem.

1b) Diffusion Problem with Constant Source Boundary Condition[2] (val-1b.inp)

Diffusion of tritium through a semi-infinite SiC layer is modelled with a constant source located on one boundary. No solubility or trapping is included. The concentration as a function of time and position is given by

$$C = C_o \, erfc\left(\frac{x}{2\sqrt{Dt}}\right) \tag{2}$$

Comparison of the TMAP4 results on an IBM PS 2/70 and the analytical solution developed using Lotus 123™ Version 3.0, taking 26 terms in the series solution for $erfc(x)$, is given in Table 12 as a function of time at x = 0.2 mm. For simplicity, both the diffusion coefficient and the initial concentration were set to unity. Agreement between

the code predictions and Equation (2) is very good with TMAP4 overpredicting the concentration by less than 1% for times greater than one second.

TABLE 12 COMPARISON OF TMAP4 AND ANALYTIC SOLUTION FOR
DIFFUSION PROBLEM WITH CONSTANT SOURCE BOUNDARY CONDITION:
CONCENTRATION HISTORY AT X = 0.2 M

Time	TMAP4	Theory	Variation
0	0	0	0
1	0.85969	0.887537	-0.03138
2	0.92516	0.920344	0.005232
3	0.94379	0.934925	0.009482
4	0.95315	0.943628	0.010091
5	0.95901	0.949571	0.00994
6	0.96312	0.95396	0.009602
7	0.96622	0.957372	0.009242
8	0.96866	0.960122	0.008892
9	0.97067	0.962401	0.008592
10	0.97235	0.964329	0.008317
11	0.97379	0.965988	0.008076
12	0.97506	0.967436	0.007881
13	0.97618	0.968712	0.007709
14	0.97717	0.96985	0.007548
15	0.97808	0.970872	0.007424
16	0.97889	0.971796	0.007299
17	0.97964	0.972638	0.007199
18	0.98032	0.973409	0.0071
19	0.98095	0.974118	0.007014
20	0.98153	0.974773	0.006932
21	0.98207	0.975381	0.006858
22	0.98257	0.975947	0.006787
23	0.98303	0.976475	0.006713
24	0.98345	0.97697	0.006632
25	0.98385	0.977435	0.006563
26	0.98422	0.977874	0.00649
27	0.98457	0.978287	0.006422
28	0.98489	0.978678	0.006347
29	0.9852	0.979049	0.006283
30	0.98548	0.979401	0.006207

As a second check, the concentration as a function of position at a give time, t = 25 s, from TMAP4 was compared with Equation (2). Results are given in Table 13. Here the variation is seen to be smaller for small distances, x, from the surface but it increases as x increases. This is shown graphically in Figure 2.

TABLE 13 COMPARISON OF TMAP4 WITH THE ANALYTIC SOLUTION FOR SEMI-INFINITE SLAB WITH CONSTANT SOURCE: CONCENTRATION PROFILE FOR T = 25 S

x (m)	TMAP4	Theory	Variation
0	1	1	0
0.05	0.99462	0.994358	0.000263
0.15	0.98385	0.983076	0.000788
0.25	0.97309	0.971796	0.001331
0.35	0.96234	0.960523	0.001892
0.45	0.95159	0.949257	0.002458
0.55	0.94086	0.938002	0.003047
0.65	0.93014	0.926759	0.003649
0.75	0.91944	0.91553	0.004271
0.85	0.90876	0.904318	0.004912
0.95	0.8981	0.893126	0.00557
1.05	0.88747	0.881954	0.006254
1.15	0.87686	0.870806	0.006952
1.25	0.86629	0.859684	0.007684
1.35	0.85574	0.848589	0.008427
1.45	0.84523	0.837524	0.0092
1.55	0.83476	0.826492	0.010004
1.65	0.82433	0.815493	0.010836
1.75	0.81394	0.804531	0.011695
1.85	0.8036	0.793607	0.012592
1.95	0.7933	0.782723	0.013512

Semi-infinite Constant Source Model
SQAP Reference 4.2.1.b
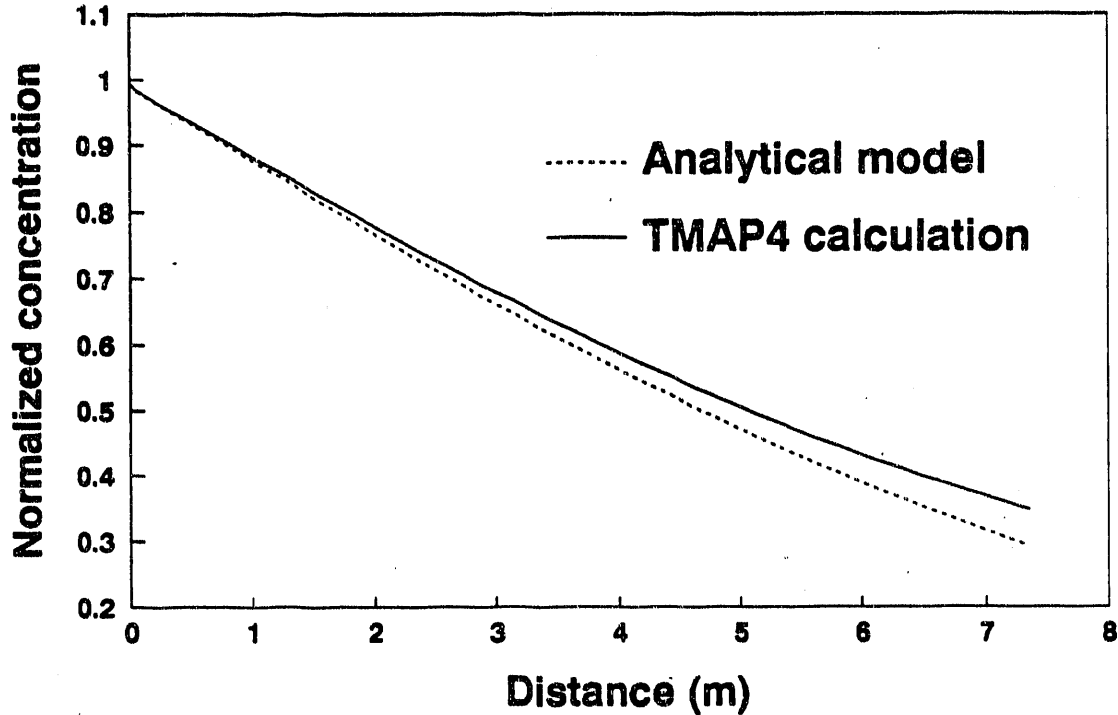
Figure 2. Concentration profile at t = 25 s for semi-infinite slab with constant source.

Finally, the diffusive flux, was compared with the analytic solution where the flux is proportional to the derivative of the concentration with respect to x and is given by

$$J = C_o \sqrt{\frac{D}{\pi t}} \exp\left(\frac{x}{2\sqrt{Dt}}\right) \tag{3}$$

The flux as given by Equation (3) is compared with values calculated by TMAP4 in Table 14. The diffusivity, D, and the initial concentration, C_o, were both taken as unity, and the distance, x, was taken as zero in this comparison. TMAP4 initially overpredicts because of the finite time step (1 second in this case). That may be reduced by making the time step smaller. Results are shown graphically in Figure 3.

28

TABLE 14 COMPARISON OF TMAP4 WITH THE ANALYTIC SOLUTION FOR
SEMI-INFINITE SLAB WITH CONSTANT SOURCE:
FLUX RATE INTO THE SURFACE

Time (s)	TMAP4	Theory	Variance
0	1	1	0
1	0.99875	0.56419	0.770238
2	0.50062	0.398942	0.254868
3	0.37514	0.325735	0.151672
4	0.31254	0.282095	0.107925
5	0.27339	0.252313	0.083534
6	0.24594	0.230329	0.067775
7	0.22528	0.213244	0.056444
8	0.20896	0.199471	0.04757
9	0.19561	0.188063	0.040129
10	0.18438	0.178412	0.033448
11	0.17473	0.17011	0.027162
12	0.16631	0.162868	0.02113
13	0.15886	0.156478	0.015222
14	0.15219	0.150786	0.009311
15	0.14618	0.145673	0.00348
16	0.14073	0.141047	-0.00225
17	0.13575	0.136836	-0.00794
18	0.13119	0.132981	-0.01347
19	0.12699	0.129434	-0.01888
20	0.12313	0.126157	-0.02399
21	0.11955	0.123116	-0.02897
22	0.11624	0.120286	-0.03363
23	0.11317	0.117642	-0.03801
24	0.11031	0.115165	-0.04215
25	0.10766	0.112838	-0.04589
26	0.10518	0.110647	-0.04941
27	0.10287	0.108578	-0.05257
28	0.10071	0.106622	-0.05545
29	0.098693	0.104767	-0.05798
30	0.096801	0.103006	-0.06024
31	0.095027	0.101331	-0.06222
32	0.09336	0.099736	-0.06392
33	0.091792	0.098213	-0.06538
34	0.090316	0.096758	-0.06658
35	0.088924	0.095365	-0.06754
36	0.08761	0.094032	-0.06829
37	0.086368	0.092752	-0.06883
38	0.085191	0.091524	-0.06919
39	0.084076	0.090343	-0.06937
40	0.083017	0.089206	-0.06938

Semi-infinite Constant Source Model
SQAP Reference 4.2.1.b
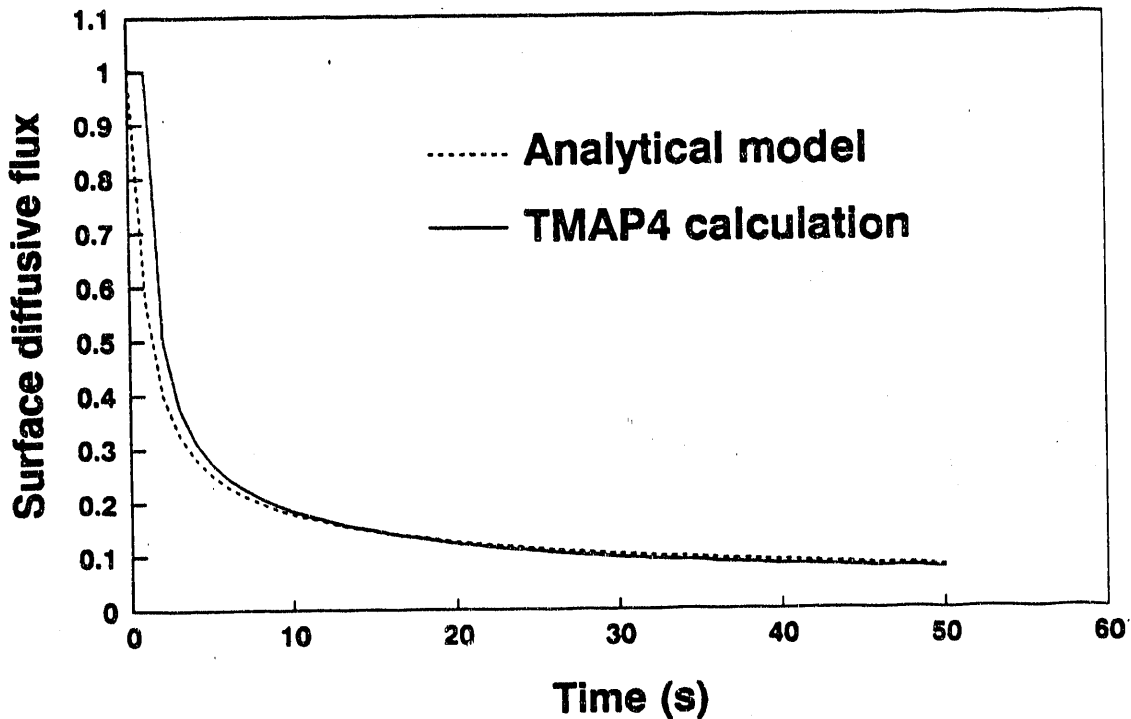
Figure 3. Comparison of TMAP4 calculation with the analytical solution for the flux into a semi-infinite slab with constant source.

1c) Diffusion Problem with Partially Preloaded Slab[2] (val-1c.inp)

Diffusion of tritium through a semi-infinite SiC layer is modelled with an initial loading of 1 atom/m^3 in the first 10 m of a 2275-m slab. Solubility is unity and no trapping is included. The analytical solution is given by

$$C = \frac{C_o}{2}\left[erf\left(\frac{h-x}{2}\sqrt{Dt}\right) + erf\left(\frac{h+x}{2\sqrt{Dt}}\right)\right] \tag{4}$$

where h is the thickness of the pre-loaded portion of the layer. The results for the concentration are shown in Table 15 as a function of time at x = 12 m. Note that this is

obtained by taking the average of mobile species concentration values at x=11.5 m (node 12) and x=12.5 m (node 13) from the problem *.out file.

TABLE 15 COMPARISON OF TMAP4 WITH THE ANALYTIC SOLUTION FOR DIFFUSION PROBLEM WITH PARTIALLY PRE-LOADED SLAB AT X = 12 M

Time (s)	TMAP4	Theory	Variance
0	0.000000	0.000000	0.0000
5	0.261690	0.263545	-0.0070
10	0.326515	0.327360	-0.0026
15	0.356960	0.357500	-0.0015
20	0.375270	0.375663	-0.0010
25	0.387370	0.387717	-0.0009
30	0.395545	0.395872	-0.0008
35	0.400950	0.401260	-0.0008
40	0.404285	0.404578	-0.0007
45	0.406045	0.406317	-0.0007
50	0.406585	0.406837	-0.0006
55	0.406185	0.406414	-0.0006
60	0.405060	0.405261	-0.0005
65	0.403360	0.403545	-0.0005
70	0.401235	0.401397	-0.0004
75	0.398775	0.398917	-0.0004
80	0.396065	0.396188	-0.0003
85	0.393160	0.393274	-0.0003
90	0.390125	0.390224	-0.0003
95	0.386995	0.387079	-0.0002
100	0.383800	0.383871	-0.0002

The maximum variation is seen to occur at the initiation of the analysis with TMAP4 underpredicting the concentration by about 0.7%. However, within a short time this difference approaches zero, and the calculation is correct to three significant figures. Error functions were calculated using Lotus 123™ and including 26 terms in the series solution for arguments less than 3.0.

At the surface (x = 0) the concentration is given by

$$C = C_o \; erf\left(\frac{h}{2\sqrt{Dt}}\right) \tag{5}$$

while at x = h its value is described by

$$C = \frac{C_o}{2} \; erf\left(\frac{h}{\sqrt{Dt}}\right) \tag{6}$$

Tables 16 and 17 list the analytical solutions for Equations (5) and (6) along with their TMAP4-calculated counterparts. Differences between the analytical solutions and the calculated values are virtually non-existent over the length of time being analyzed. Again TMAP4 was run on an IBM PS 2/70. The theory was evaluated as a series in Lotus 123™ discarding terms of order 1.0E-14 and smaller.

TABLE 16 COMPARISON OF TMAP4 AND ANALYTICAL SOLUTION FOR CONCENTRATION HISTORY AT x=0 IN A PARTIALLY PRELOADED SEMI-INFINITE SLAB

Time (s)	TMAP4	Theory	Variance
0	1	1	0.000000
5	0.99752	0.998435	-0.000916
10	0.9731	0.974653	-0.001593
15	0.93114	0.932111	-0.001042
20	0.88569	0.886154	-0.000523
25	0.84255	0.842701	-0.000179
30	0.80333	0.803294	0.000044
35	0.76814	0.768002	0.000179
40	0.73664	0.736448	0.000261
45	0.70839	0.708159	0.000326
50	0.68293	0.682689	0.000352
55	0.65989	0.659644	0.000373
60	0.63893	0.63869	0.000376
65	0.61978	0.619545	0.000380
70	0.60221	0.601975	0.000390
75	0.58601	0.585784	0.000386
80	0.57102	0.570805	0.000377
85	0.55711	0.556898	0.000381
90	0.54414	0.543943	0.000361
95	0.53203	0.53184	0.000357
100	0.52068	0.5205	0.000346

Time (s)	TMAP4	Theory	Variance
0	0.5	0.500000	0.000000
5	0.5	0.500000	0.000000
10	0.49999	0.500000	-0.000020
15	0.49982	0.499870	-0.000099
20	0.4991	0.499217	-0.000235
25	0.49749	0.497661	-0.000344
30	0.49489	0.495088	-0.000401
35	0.49138	0.491586	-0.000420
40	0.48713	0.487326	-0.000403
45	0.48231	0.482493	-0.000378
50	0.477085	0.477250	-0.000345
55	0.471595	0.471735	-0.000296
60	0.465935	0.466055	-0.000258
65	0.460195	0.460295	-0.000217
70	0.45443	0.454516	-0.000188
75	0.448695	0.448765	-0.000155
80	0.44302	0.443077	-0.000128
85	0.43743	0.437477	-0.000106
90	0.43195	0.431981	-0.000073
95	0.426575	0.426603	-0.000067
100	0.42133	0.421350	-0.000048

1d) Permeation Problem with Trapping[2] (val-1da.inp, val-1db.inp)

This validation problem models permeation through a membrane with a constant source in which traps are operative. The breakthrough time may have one of two limiting values depending on whether the trapping is in the *effective diffusivity* or *strong-trapping* regime.[3] A trapping parameter is defined by

$$\zeta = \frac{\lambda^2 v}{\rho D_o} \exp\left(\frac{E_d - e}{kT}\right) + \frac{c}{\rho} \qquad (7)$$

where

λ = lattice parameter

v = Debye frequency ($\approx 10^{13}$ s^{-1})

ρ = trapping site fraction

D_o = diffusivity pre-exponential

E_d = diffusion activation energy

ϵ = trap energy

k = Boltzmann's constant

T = temperature

c = dissolved gas atom fraction.

The descriminant for which regime is dominant is the ratio of ζ to c/ρ. If $\zeta \gg c/\rho$ then the effective diffusivity regime applies, and the permeation transient is identical to the standard diffusion transient but with the diffusivity replaced by an effective diffusivity,

$$D_{eff} = \frac{D}{1 + \dfrac{1}{\zeta}} \quad . \tag{8}$$

In this limit, the breakthrough time, defined as the intersection of the steepest tangent to the diffusion transient with the time axis, will be

$$\tau_{b_e} = \frac{l^2}{2\,\pi^2\,D_{eff}} \quad . \tag{9}$$

where l is the thickness of the slab and D is the diffusivity of the gas through the material. The permeation transient is then given by

$$J_p = \frac{c_o D}{l} \left\{ 1 + 2\sum_{m=1}^{\infty} \left[(-1)^m \exp\left(-2m^2 \frac{t}{\tau_{b_e}} \right) \right] \right\} \tag{10}$$

where τ_{b_e} is as defined in Equation (9).

In the deep-trapping limit, $\zeta \ll c/\rho$, and no permeation occurs until essentially all the traps have been filled. Then permeation rapidly turns on to its steady state value. The breakthrough time is given by

$$\tau_{b_d} = \frac{l^2 \rho}{2c_o D} \tag{11}$$

where c_o is the steady dissolved gas concentration at the upstream ($x = 0$) side.

We exercised TMAP4 in both these limits with an upstream-side starting concentration of 0.0001 atom fraction, a diffusivity of 1 m^2/s, a trapping site fraction of 0.1, $\lambda^2 = 10^{-15}$ m^2, and a temperature of 1000 K. For the effective diffusivity limit, we selected $\epsilon/k = 100$ K to give $\zeta = 90.48$ c/ρ. For the deep trapping limit we took $\epsilon/k = 10000$ K to give $\zeta = 0.04533$ c/ρ. Aside from the coarser convergence limit required to run the strong-trapping model, there were no other differences in the input files. The results are presented in Figures 4 and 5.

Effective-Diffusivity Trapping in a Slab
SQAP Reference 4.2.1.d
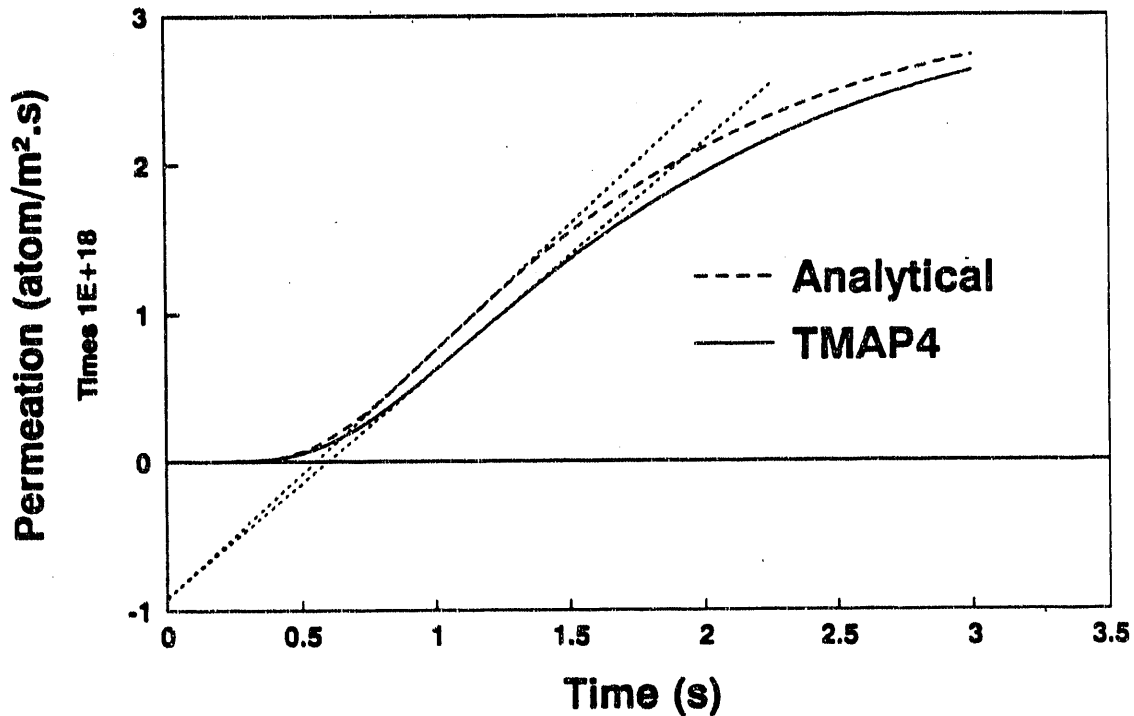
Figure 4. Permeation history for a slab subject to effective-diffusivity limit trapping.

Notice that in neither case is the behavior "ideal" in the sense that the calculated transient differs somewhat from the theoretical one for the limiting case. Such deviation is to be expected because in neither case was the actual problem ideal. In Figure 4 for the effective-diffusivity behavior, the breakthrough time in the calculation is 0.5917 seconds as compared with a theoretical value of 0.5599 seconds. However, the effects of trapping are clearly evident because the breakthrough time in the absence of trapping would have been 0.0506 seconds for the same parameters otherwise. In Figure 5 note that the permeation turns on much more abruptly than in Figure 4, and it agrees quite well with the breakthrough time of 500 seconds calculated by Equation (11). There is some diffusive permeation before the theoretical breakthrough time and it takes a while

Strong Trapping in a Slab
SQAP Reference 4.2.1.d
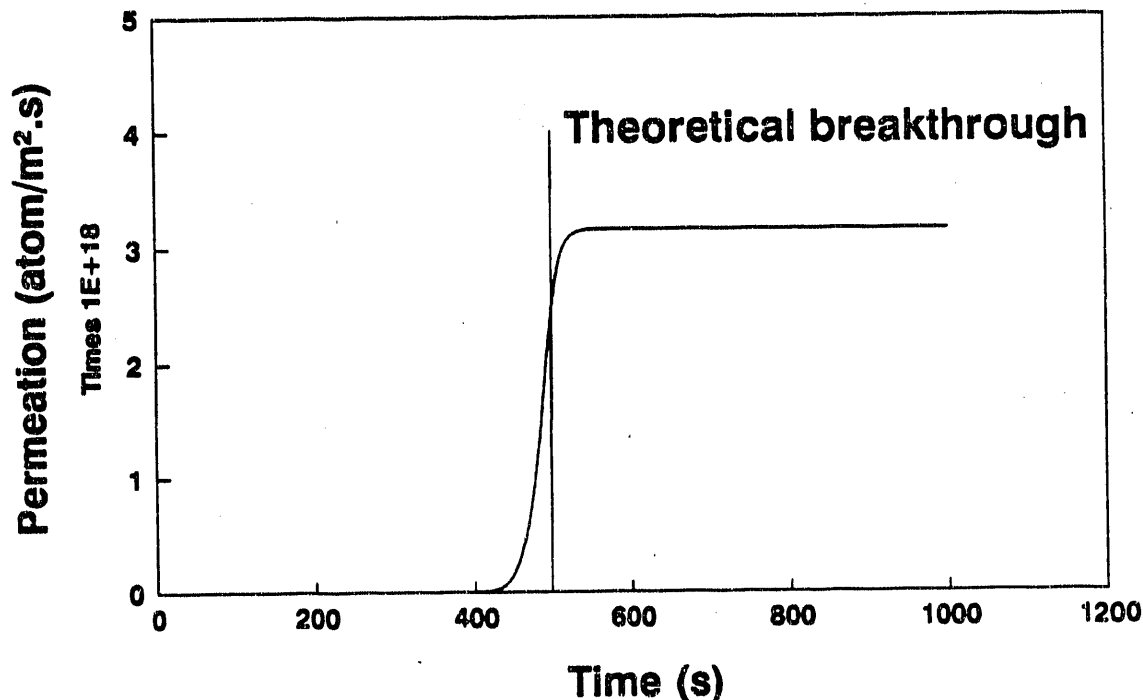
Figure 5. Permeation transient in a slab subject to strong-trapping.

to saturate after breakthrough. However, the general characteristics in both cases are in good agreement with the theory.

1e) Diffusion Problem with Composite Material Layers[2] (val-1e.inp)

A composite layer of PyC and SiC is modelled with a constant concentration boundary condition on the surface of the PyC. The concentration in the second layer (SiC) of this composite can be found from the following expression

$$C = C_o \frac{D_{PyC}(a-x)}{aD_{PyC}+lD_{SiC}}$$

$$-2C_o \sum_{n=1}^{\infty} \frac{\sin(l\beta_n)\sin(ka\beta_n)\sin[k(a-x)\beta_n]}{\beta_n\left[l\sin^2(ka\beta_n)+\sigma ka\sin^2(l\beta_n)\right]} \exp\left(-D_{PyC}\beta_n^2 t\right)$$

(12)

where

a = thickness of PyC

l = thickness of SiC

$$k = \sqrt{\frac{D_{PyC}}{D_{SiC}}}$$

$$\sigma = \frac{1}{k}$$

and β_n are the roots of

$$\cot(\beta l) + \sigma\cot(k\beta a) = 0 \ .$$

The TMAP4 calculated concentration for x = 8 μm is compared to the solution given by Equation (12) for a case where a = 33 μm, l = 63 μm in Table 18. The agreement is very good, although TMAP4 underpredicts slightly at short times. The agreement is better than 0.1% over most of the interval of comparison and is better than 5% everywhere. The same comparison is made graphically in Figure 6.

TABLE 18 COMPARISON OF TMAP4 AND ANALYTICAL SOLUTION FOR CONCENTRATION HISTORY (ATOM/M³) AT X=8 MICROMETERS IN A COMPOSITE MATERIAL

Time (s)	TMPA4	Theory	Variance
0	0	0	0
5	1,80950e+25	1.89284e+25	-0.04403
10	2.14600e+25	2.18703e+25	-0.01876
15	2.25380e+25	2.27425e+25	-0.00899
20	2.29160e+25	2.30083e+25	-0.00401
25	2.30510e+25	2.30894e+25	-0.00166
30	2.30990e+25	2.31142e+25	-0.00066
35	2.31160e+25	2.31217e+25	-0.00025
40	2.31220e+25	2.31240e+25	-0.00009
45	2.31240e+25	2.31247e+25	-0.00003
50	2.31250e+25	2.31249e+25	0.00000

Diffusion in Composite Material Layers
SQAP Reference 4.2.1.e
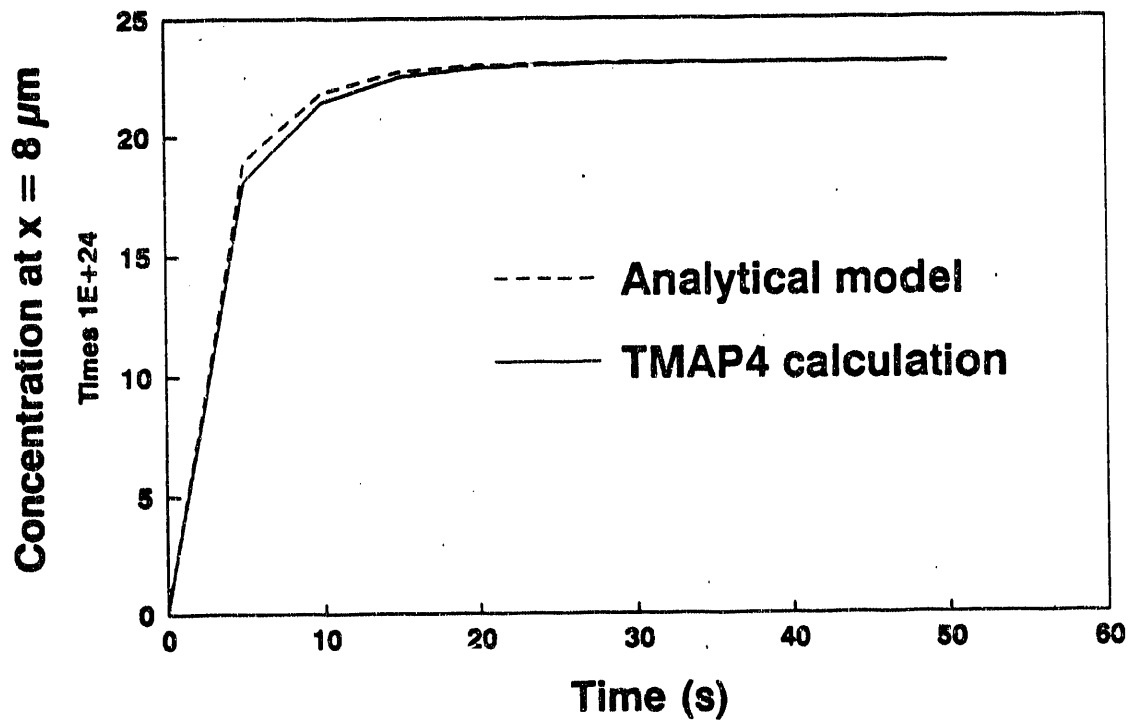
Figure 6. Comparison of TMAP4 results with theory for concentration build-up by diffusion in a composite-layer material with a constant source on one side.

39

1f) Heat Sink/Source Problem (val-1fa.inp, val-1fb.inp)

The heat transfer calculation capability of the TMAP4 code is validated using two
cases. The first case examines TMAP4's thermal capabilities by modelling heat
conduction in a slab having internal heat generation. An adiabatic surface is applied to
one side of the layer while a constant temperature is imposed on the other surface. The
analytical solution for this case is given by

$$T = T_s + \frac{QL^2}{2k}\left(1 - \frac{x^2}{L^2}\right) \tag{13}$$

where

Q = internal heat generation rate

L = thickness of the layer

κ = thermal conductivity

T_s = imposed surface temperature.

Table 19 compares the calculated temperature as a function of position between TMAP4
results and Equation (13) for $Q = 1.0 \times 10^4$ W/m^3, $L = 1.6$ m, $\kappa = 10$ W/m.K, and
$T_s = 300$ K. We also use $\rho C_p = 1$ J/m^3.K, for a thermal time constant of 26 ms, and

TABLE 19 COMPARISON OF TMAP4 AND ANALYTICAL SOLUTION FOR
HEAT SINK/SOURCE PROBLEM WITH INTERNAL HEAT GENERATION

Position (m)	TMAP4	Theory	Variance
0	1580	1580	0
0.1	1580	1575	0.003175
0.3	1540	1535	0.003257
0.5	1460	1455	0.003436
0.7	1340	1335	0.003745
0.9	1180	1175	0.004255
1.1	980	975	0.005128
1.3	740	735	0.006803
1.5	460	455	0.010989
1.6	300	300	0

an elapsed time of 50 seconds. At that time steady state has been reached. As may be seen in Table 19, the agreement is excellent.

In a second case an effective mass diffusivity is used to simulate a thermal transient. In that instance temperature is held constant, but the mass-diffusion transient is taken as an analog for the thermal transient. The same geometry is assumed, except that the thickness, L, is only 0.375 m. The general equation is

$$T(x,t) = T_o + (T_1 - T_o)\left[1 - \frac{2}{\pi} \sum_{m=0}^{\infty} \frac{(-1)^m}{\left(m + \frac{1}{2}\right)} \cos(\gamma_m x)\exp\left(-\alpha \gamma_m^2 t\right)\right] \tag{14}$$

where

$$\gamma_m = \left(m + \frac{1}{2}\right)\frac{\pi}{L}$$

and

$$\alpha = \frac{k}{\rho C_p}$$

is the thermal diffusivity. By substituting temperatures for concentrations and the thermal diffusivity for the mass diffusivity, we complete the analog solution. Here, $\alpha = 1.29035 \times 10^{-3}$ m²/s, $T_o = 300$ K, and $T_1 = 373$ K. Table 20 compares the TMAP4 results at $x = 0$ with those of Equation (14). Again, the agreement is very good.

1g) Simple Chemical Reaction Problem (val-1ga.inp, val-1gb.inp)

A simple time-dependent chemical reaction given by

$$A + B \rightarrow AB \tag{15}$$

is modelled in a functional enclosure. The reaction rate, R_c, is positive if the species AB is being produced in the reaction and negative if it is being consumed. The forward rate coefficient, K_R, for the reaction has no spatial or time dependence. The reaction rate is

Time (s)	TMAP4	Theory	Variance
0	300	300	0
10	305.4	302.8584	0.008392
20	314.25	314.427	-0.00056
30	323.69	325.9433	-0.00691
40	332.28	335.4314	-0.0094
50	339.62	343.037	-0.00996
60	345.72	349.1069	-0.0097
70	350.73	353.9476	-0.00909
80	354.83	357.8077	-0.00832
90	358.18	360.8857	-0.0075
100	360.92	363.3401	-0.00666
110	363.15	365.2973	-0.00588
120	364.96	366.8579	-0.00517
130	366.45	368.1023	-0.00449
140	367.65	369.0946	-0.00391
150	368.64	369.8858	-0.00337
160	369.45	370.5168	-0.00288
170	370.1	371.0199	-0.00248
180	370.64	371.4211	-0.0021

$$R_c = K_r \, C_A \, C_B \tag{16}$$

The analytical solution for the concentration of species AB is the function

$$C_{AB} = C_{B_0} \frac{1 - \exp\left[K_R t\left(C_{B_0} - C_{A_0}\right)\right]}{1 - \dfrac{C_{B_0}}{C_{A_0}} \exp\left[K_R t\left(C_{B_0} - C_{A_0}\right)\right]} \tag{17}$$

where

C_{AB} = concentration of species AB

C_{A_0} = initial concentration of species A

C_{B_0} = initial concentration of species B

In the special case when C_{A_0} and C_{B_0} are equal, this becomes

$$C_{AB} = C_{A_0} - \cfrac{1}{\cfrac{1}{C_{A_0}} + K_R t} \qquad\qquad (18)$$

We exercised TMAP4 under each of these conditions. Table 21 gives a numerical comparison of the values computed by TMAP4 when the starting pressure of species A and B were both 1.0 μPa, and K_R was 4.14×10^{-15} molecule.m^3/atom^2.s. The calculation and theoretical value are in excellent agreement. Table 22 gives the comparison for the same input file but with C_{B_0} reduced to 0.1 μPa. These are shown graphically in Figure 7. The distinction between the TMAP4 values and the analytical results vanishes.

Simple Chemical Reaction Problem
SQAP Reference 4.2.1.g
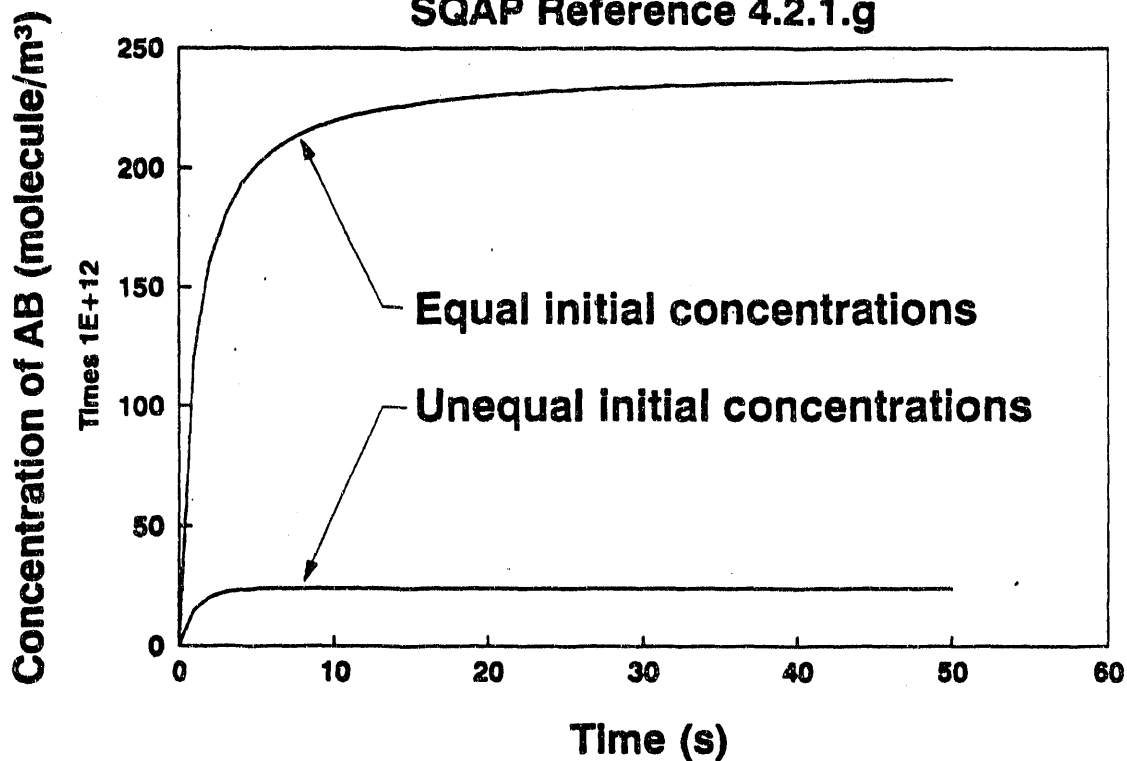
Figure 7. TMAP4 calculations agreed well with theoretical values for both equal and unequal starting reactant concentrations.

43

TABLE 21 COMPARISON OF TMAP4 AND ANALYTICAL RESULTS FOR
SIMPLE CHEMICAL REACTION PROBLEM WITH EQUAL STARTING CONCENTRATIONS

Time (s)	TMAP4	Theory	Variance
0	0	0	0
1	1.2036e+14	1.2077e+14	-0.0034186
2	1.6074e+14	1.6103e+14	-0.0018041
3	1.8095e+14	1.8116e+14	-0.0011555
4	1.9308e+14	1.9324e+14	-0.0008105
5	2.0117e+14	2.0129e+14	-0.000587
6	2.0694e+14	2.0704e+14	-0.0004794
7	2.1127e+14	2.1135e+14	-0.0003906
8	2.1464e+14	2.1471e+14	-0.0003138
9	2.1734e+14	2.1739e+14	-0.0002356
10	2.1954e+14	2.1959e+14	-0.0002144
11	2.2138e+14	2.2142e+14	-0.000167
12	2.2293e+14	2.2297e+14	-0.0001585
13	2.2426e+14	2.2429e+14	-0.000145
14	2.2541e+14	2.2544e+14	-0.0001452
15	2.2642e+14	2.2645e+14	-0.0001289
16	2.2731e+14	2.2734e+14	-0.0001197
17	2.2811e+14	2.2813e+14	-0.0000727
18	2.2881e+14	2.2883e+14	-0.0000999
19	2.2945e+14	2.2947e+14	-0.0000806
20	2.3003e+14	2.3004e+14	-0.0000592
21	2.3055e+14	2.3057e+14	-0.0000713
22	2.3103e+14	2.3104e+14	-0.0000597
23	2.3147e+14	2.3148e+14	-0.0000492
24	2.3187e+14	2.3188e+14	-0.0000602
25	2.3224e+14	2.3226e+14	-0.0000671
26	2.3259e+14	2.3260e+14	-0.0000415
27	2.3291e+14	2.3292e+14	-0.0000393
28	2.3321e+14	2.3322e+14	-0.0000284
29	2.3349e+14	2.3349e+14	-0.0000183
30	2.3375e+14	2.3375e+14	-0.0000171
31	2.3399e+14	2.3400e+14	-0.000032
32	2.3422e+14	2.3423e+14	-0.0000266
33	2.3443e+14	2.3444e+14	-0.0000491
34	2.3464e+14	2.3464e+14	-0.0000191
35	2.3483e+14	2.3484e+14	-0.0000264
36	2.3501e+14	2.3502e+14	-0.0000321
37	2.3518e+14	2.3519e+14	-0.0000397
38	2.3535e+14	2.3535e+14	-0.0000098
39	2.3550e+14	2.3551e+14	-0.0000304
40	2.3565e+14	2.3565e+14	-0.0000188

TABLE 22 COMPARISON OF TMAP4 AND ANALYTICAL RESULTS FOR SIMPLE CHEMICAL REACTION PROBLEM WITH UNEQUAL STARTING CONCENTRATIONS

Time (s)	TMAP4	Theory	Variance
0	0	0	0
1	1.4897e+13	1.4942e+13	-0.0029806
2	2.0468e+13	2.0501e+13	-0.0015964
3	2.2664e+13	2.2684e+13	-0.0008687
4	2.3549e+13	2.3559e+13	-0.0004227
5	2.3908e+13	2.3913e+13	-0.0002012
6	2.4054e+13	2.4056e+13	-0.0000976
7	2.4113e+13	2.4115e+13	-0.0000685
8	2.4138e+13	2.4138e+13	-0.0000144
9	2.4148e+13	2.4148e+13	0.00000078
10	2.4152e+13	2.4152e+13	0.00000426
11	2.4153e+13	2.4153e+13	-0.0000203
12	2.4154e+13	2.4154e+13	-0.0000057
13	2.4154e+13	2.4154e+13	-0.0000165
14	2.4155e+13	2.4155e+13	0.00002042
15	2.4155e+13	2.4155e+13	0.00001862
16	2.4155e+13	2.4155e+13	0.00001789
17	2.4155e+13	2.4155e+13	0.00001759
18	2.4155e+13	2.4155e+13	0.00001747
19	2.4155e+13	2.4155e+13	0.00001742
20	2.4155e+13	2.4155e+13	0.0000174
21	2.4155e+13	2.4155e+13	0.00001739
22	2.4155e+13	2.4155e+13	0.00001739
23	2.4155e+13	2.4155e+13	0.00001739
24	2.4155e+13	2.4155e+13	0.00001739
25	2.4155e+13	2.4155e+13	0.00001739

1h) System (Multiple Enclosure Volumes) Problem (val-1h.inp)

A three-enclosure model is presented having a known convective outflow from one enclosure to the next. The first enclosure is a boundary enclosure with a constant concentration of the species "t2". The flux, $\overline{j}$, of molecules into the first functional enclosure (number 2) is given by

$$\bar{j} = QC_1 \qquad (19)$$

where

Q = volumetric flow rate, common through the enclosures

C_1 = constant concentration in enclosure 1.

Gas from the first enclosure flows into the second and ultimately into the third with both enclosures 2 and 3 having initial concentrations of zero. Concentrations of particles in both functional enclosures 2 and 3 are found as a function of time. The analytical solution consists of the two simultaneous equations:

$$\frac{\partial C_2}{\partial t} = \frac{Q(C_1 - C_2)}{V_2} \qquad (20)$$

$$\frac{\partial C_3}{\partial t} = \frac{Q(C_2 - C_3)}{V_3} \qquad (21)$$

Solutions to this set with the initial condition that $C_{2_0} = C_{3_0} = 0$ are

$$C_2 = C_1 \left[1 - \exp\left(-\frac{Qt}{V_2}\right) \right] \qquad (22)$$

and

$$C_3 = C_1 \left[1 - \left(1 + \frac{Qt}{V}\right) \exp\left(\frac{Qt}{V}\right) \right] \qquad (23)$$

if $V_2 = V_3 = V$ or

$$C_3 = C_1 \left[1 - \frac{V_2}{V_2 - V_3} \exp\left(-\frac{Qt}{V_2}\right) + \frac{V_3}{V_2 - V_3} \exp\left(-\frac{Qt}{V_3}\right) \right] \qquad (24)$$

otherwise. These equations were solved using Lotus 123™ for volumes of 1 m³ for each enclosure, and an inlet "t2" partial pressure of 1 Pa. Graphical comparison of results is given in Figure 8 where it is impossible to distinguish between the TMAP4 calculation

and the theoretical result. The data are listed along with variances between TMAP4 and Lotus solutions in Table 23.

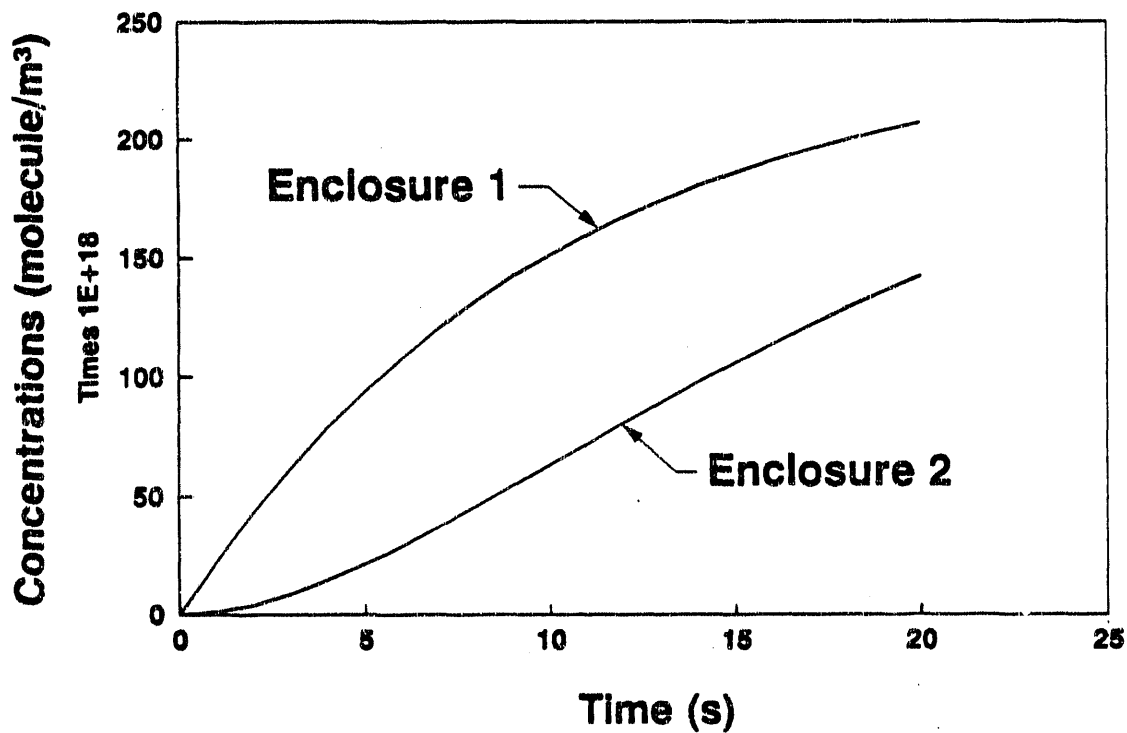## Multiple Enclosure Chamber Problem
SQAP Reference 4.2.1.h

Figure 8. There is virtually no difference between TMAP4 calculations and analytical results for the case of concentration transients in multiple chambers.

TABLE 23 COMPARISON OF TMAP4 AND ANALYTICAL RESULTS FOR A MULTIPLE ENCLOSURE PROBLEM

Time (s)	Enclosure 2			Enclosure 3		
	TMAP4	Theory	Variance	TMAP4	Theory	Variance
0	0	0	0	0	0	0
1	2.2748e+19	2.2759e+19	-0.0004619	1.1287e+18	1.1190e+18	0.0087015
2	4.3332e+19	4.3351e+19	-0.0004444	4.2064e+18	4.1907e+18	0.00374194
3	6.1958e+19	6.1984e+19	-0.0004253	8.8521e+18	8.8335e+18	0.00210936
4	7.8812e+19	7.8844e+19	-0.0004094	1.4740e+19	1.4720e+19	0.00133206
5	9.4064e+19	9.4100e+19	-0.0003801	2.1591e+19	2.1573e+19	0.00085062
6	1.0786e+20	1.0790e+20	-0.0004032	2.9169e+19	2.9153e+19	0.00054186
7	1.2035e+20	1.2039e+20	-0.0003625	3.7274e+19	3.7261e+19	0.00033855
8	1.3165e+20	1.3170e+20	-0.0003431	4.5737e+19	4.5728e+19	0.00019407
9	1.4188e+20	1.4192e+20	-0.0002906	5.4416e+19	5.4412e+19	0.00007801
10	1.5113e+20	1.5117e+20	-0.0002921	6.3194e+19	6.3194e+19	-0.0000051
11	1.5950e+20	1.5955e+20	-0.0002918	7.1974e+19	7.1978e+19	-0.0000605
12	1.6708e+20	1.6712e+20	-0.0002525	8.0676e+19	8.0684e+19	-0.0000996
13	1.7393e+20	1.7398e+20	-0.0002698	8.9234e+19	8.9247e+19	-0.0001428
14	1.8014e+20	1.8018e+20	-0.0002184	9.7598e+19	9.7615e+19	-0.0001725
15	1.8575e+20	1.8579e+20	-0.0002235	1.0573e+20	1.0575e+20	-0.0001686
16	1.9083e+20	1.9087e+20	-0.0002077	1.1359e+20	1.1361e+20	-0.0002171
17	1.9543e+20	1.9546e+20	-0.0001765	1.2117e+20	1.2119e+20	-0.0001845
18	1.9959e+20	1.9962e+20	-0.0001609	1.2844e+20	1.2846e+20	-0.0001923
19	2.0335e+20	2.0338e+20	-0.0001675	1.3539e+20	1.3542e+20	-0.0002303
20	2.0676e+20	2.0679e+20	-0.0001355	1.4202e+20	1.4206e+20	-0.000254

Comparison with Experiments

The second phase of code validation is the comparison of code results with actual experimental data. Three experimental data sets were selected for modelling. Each was published in a refereed journal.

2a) Ion Implantation Experiment (val-2a.inp)

This problem is the simulation of experimental results obtained at the INEL in 1985 and published.[4] The experiment involved applying an ion beam to a 2.5-cm diameter, 0.5-mm thick sample of a modified 316 stainless steel called Primary Candidate Alloy (PCA). Details of the experiment and the means of evaluating the necessary transport parameters to get a good fit between TMAP4 results and the experimental data are given in the publication. The TRIM code was used to determine that the average implantation depth for the ions was 11 μm $\pm$ 5.4 μm. Reemission data from the TRIM calculation showed that only 75% of the incident flux remained in the metal. The other 25% was re-emitted.

One known non-physical feature in the modelling is that the cleanup of the upstream surface was modelled by a simple exponential in time rather than in ion fluence which was interrupted twice during the actual experiment. The pressures upstream and downstream could have been taken as zero and obtained essentially the same results.

The plot of Figure 9 was generated. Actual experimental data are also shown on the figure. They are fairly closely approximated by the calculated permeation. Notice in the figure, however that there is a lower permeation flux value when the beam is on, and a relatively slow trail-off, compared with the calculation, when the beam was turned off. Some of this is a consequence of the experimental technique where the walls of the experimental chamber did some pumping of the gas as it came through the sample and then provided a source of deuterium when the sample permeation ceased. Some two-dimensional effects also influence the comparison.

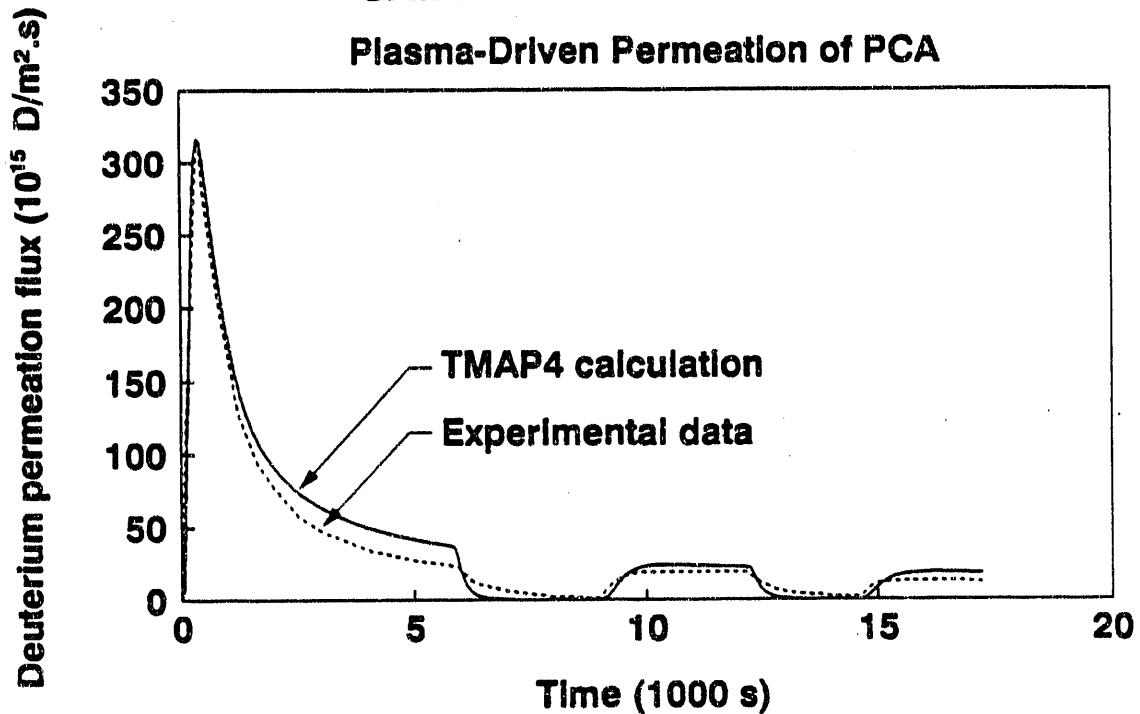# SAMPLE PROBLEM No. 1

Plasma-Driven Permeation of PCA

Figure 9. Computed permeation transient which is very similar to experimental data from an ion-implantation experiment.

2b) Material Diffusion Experiment (val-2ba.inp, val2bb.inp)

This problem is taken from work done by R. G. Macaulay-Newcombe at McMaster University.[5] He and co-workers conducted thermal absorption and desorption experiments, as well as implantation experiments, on wafers of polished beryllium. Of the several data sets presented, the one modelled here is that represented in Figure 2 (a) in their publication. The beryllium was 0.4-mm thick and had an area of 104 mm^2. It was polished to a mirror finish then exposed to 13.3 KPa of deuterium at 773 K for 50 minutes. It was quickly cooled under a vacuum of about 1 μPa. The cooling time constant for the apparatus is taken as 45 minutes. After removing the sample from the

50

charging furnace, it was transferred in the air to a thermal desorption furnace where the temperature was increased from ambient (300 K) to 1073 K at the rate of 3 K/min. This was done under vacuum, and the pressure of the chamber was monitored by residual gas analysis and calibrated against standard leaks. In that way the emission rate from the sample could be measured as a function of temperature. Data from that measurement, given in Figure 2 (a) of their paper are reproduced in Figure 10. From Rutherford backscattering measurements made on the samples before charging with deuterium they deduced that the thickness of the oxide film was 18 nm. This is typical for polished beryllium. The metal is so reactive in air that the film forms almost immediately after any surface oxide removal. On the other hand, it is relatively stable and would only grow slightly when exposed to air between charging and thermal desorption.

This experiment is modelled using a two-segment model in TMAP4 with the segments linked. The first is the BeO film, which is modelled using 18 equally spaced nodes of 1 nm each plus the two surface nodes. The second segment is a half-thickness wafer of beryllium with reflective boundary conditions at the midplane. It is made up of 15 segments of varying thickness to accommodate solution stiffness plus the two surface nodes. The solubility of deuterium in beryllium used was that given by K. L. Wilson, et al.[6] based on work done by W. A. Swansiger, also of Sandia National Laboratory. The diffusivity of deuterium in beryllium was measured by E. Abramov, et al.[7] They made measurements on high-grade (99% pure) and extra grade (99.8% pure). The values for high-grade, consistent with Dr. Macaulay-Newcombe's measurements of the purity of his samples.

Deuterium transport properties for the BeO are more challenging. First, it is not clear in what state the deuterium exists in the BeO. However, it has been observed[8] that an activation energy of -78 kJ/mole (exothermic solution) is evident for tritium coming out of neutron irradiated beryllium in work by D. L. Baldwin of Battelle Pacific Northwest Laboratory. The same energy has appeared in other results (can be inferred from Dr. Swansiger's work cited by Wilson, et al.[6], and by R. A. Causey, et al.[9], among

51

others), so one may be justified in using it. The solubility coefficient is not well known. Measurements reported by R. G. Macaulay-Newcombe, et al.[10] and in followup telephone conversations indicate about 200 appm of D in BeO after exposure to 13.3 kPa of D_2 at 773 K. That suggests a coefficient of only 1.88×10^{18} d/m^3.Pa$^{1/2}$. On the other hand, the integrated area under the curve in the referenced experimental data is 1.1×10^{14} d/mm^2 which implies a solubility coefficient of 2.85×10^{20} d/m^3.Pa$^{1/2}$. Since much of the deuterium in the oxide layer will get out during the cool-down process (and because it gives a good fit) the solubility coefficient is taken to be 5×10^{20} d/m^3.Pa$^{1/2}$.

Deuterium diffusion measurements in BeO were made by J. D. Fowler, et al.[11] They found a wide range of results for diffusivity in BeO, depending on the physical form of the material, having measured it for single-crystal, sintered, and powdered BeO. This model uses one expression for the charging phase and another for the thermal desorption phase, believing that the surface film changed somewhat during the transfer between the two furnaces. For the charging phase the model uses 20 times that for the sintered BeO. Thermal expansion mismatches tend to open up cracks and channels in the oxide layer, so this seems a reasonable value. The same activation energy of 48.5 kJ/mole, is retained, however. For the thermal desorption phase, the prefactor of the sintered material (7×10^{-5} m^2/s) and an activation energy of 223.7 kJ/mole (53.45 kcal/mole) are used. These values give good results and lie well within the scatter of Fowler's data. Exposure of the sample to air after heating should have made the oxide more like single crystal by healing the cracks that may have developed.

The model applies 13.3 kPa of D_2 for 50 hours followed by evacuation to 1 μPa and cool down with a 45 minute time constant for one hour. The deuterium concentrations in the sample are of a complex distribution that results from first charging the sample and then discharging it during the cooldown. This problem is then restarted with different equations to simulate thermal desorption in the 1-μPa environment. That begins at 300 K and goes to 1073 K. Again, the concentration profiles in both the substrate beryllium and the oxide film have a peculiar interaction because of the activation energies involved, but the flux exuding from the sample when doubled to

account for the two sides of the specimen in the laboratory gives a good fit to the experimental data.

From the extracted diffusion species data on surface flux from the left side of thermseg/diffseg 1, the solid curve in Figure 10 is constructed where it is compared with the experimental data.
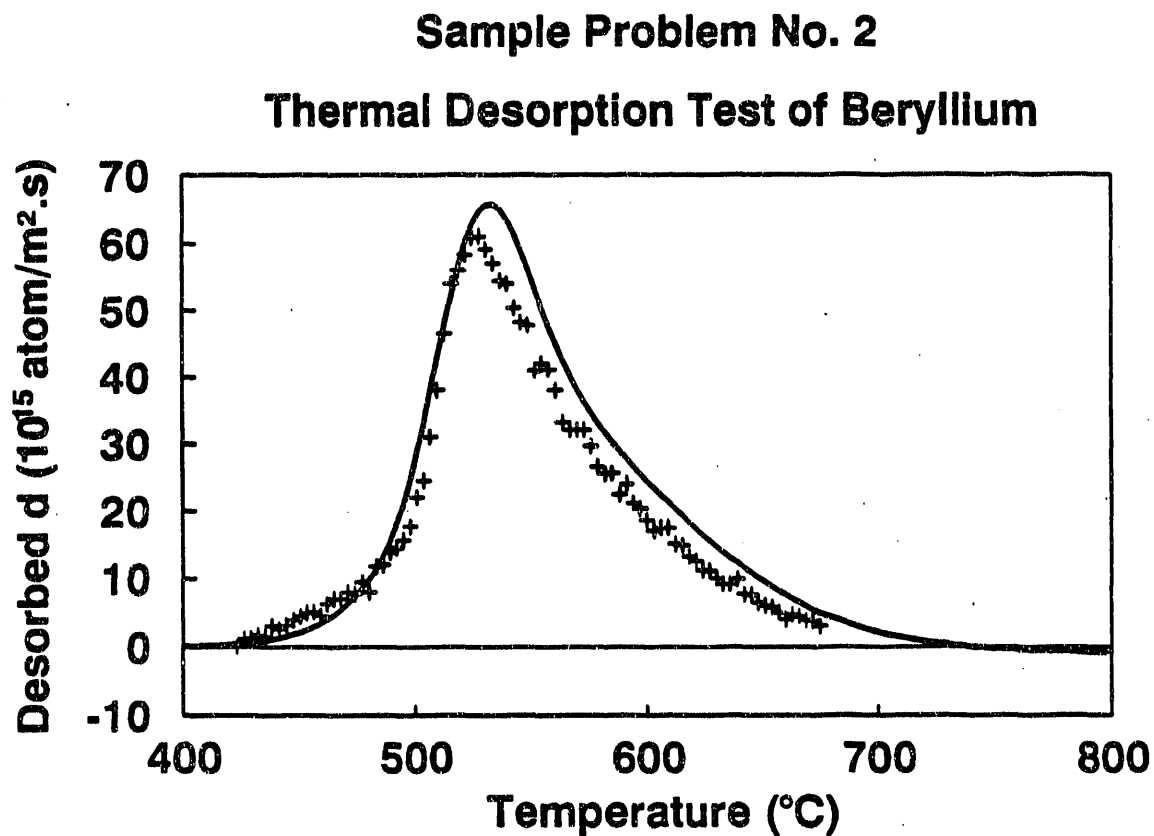
Sample Problem No. 2

Thermal Desorption Test of Beryllium

Figure 10. Comparison of calculated results (line) with experimental data (+++) for thermal desorption test of beryllium after charging for 50 hours.

2c) Test Cell Release Experiment (val-2c.inp)

This is a problem that involves multiple enclosures and chemical reactions. It is an experiment that was conducted at the Tritium Systems Test Assembly (TSTA) at Los Alamos National Laboratory and documented by Holland and Jalbert.[12] The main part of the experiment was an exposure chamber with a nominal volume of 1 m^3 which was lined with epoxy paint that is 0.16 mm thick. Tritium was admitted to the chamber as T$_2$ at the commencement of the experiment. Normally moist (20% R.H.) air was admitted to the chamber at the rate of 0.54 m^3/hr constantly throughout the test. Samples of glycol taken from a bubbler just downstream from the exposure chamber were taken at intervals and scintillation counted to determine the time averaged HTO concentration in the chamber as a histogram in time. Tritium and water were absorbed into the paint during the initial part of the test and re-emitted later. Chemical reactions described by the formulae

$$T_2 + H_2O = HTO + HT \tag{25}$$

$$HT + H_2O = HTO + H_2 \tag{26}$$
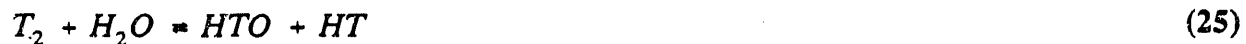
took place within the exposure chamber, mainly as a consequence of the radioactivity of the tritium itself. Results from the measurement of the resulting HTO concentration in the exposure chamber following a 10 Ci initial injection (effectively instantaneously) while purging with room air are shown in Figure 3 of the referenced article.

Modelling consists of three enclosures (1) the room from which air is drawn, (2) the exposure chamber, and (3) the tritium waste treatment system (TWT) to which the exhaust gases are directed. Only enclosure (2) is treated as "functional" or chemically active. The paint on the inside of the exposure chamber is treated as a diffusive segment with Henry's law solubility governing the concentration at its interface with enclosure (2) and non-flow conditions at the interface of the paint with the underlying aluminum foil. Experiments had previously demonstrated that there is virtually no transport of tritium into the aluminum foil. The technique for determining the constants and other

information required to generate a model that gives reasonable results are given in the paper and are not duplicated here.

Data were extracted for the HTO concentration in the exposure chamber, enclosure 2. A solid curve representing these data is compared in Figure 11 with measurements made in bubblers in line with the exposure chamber exhaust. The period over which the bubblers were active in collecting HTO from the exposure chamber is shown on the time scale. They were integrated measurements over the intervals shown. The model fits best at extended times where the intercepts with the "average-value" line segments are at the correct times. Additional uptake and release channels for short times, beyond those modelled, may be responsible for the early-time disparity.

SAMPLE PROBLEM No. 3
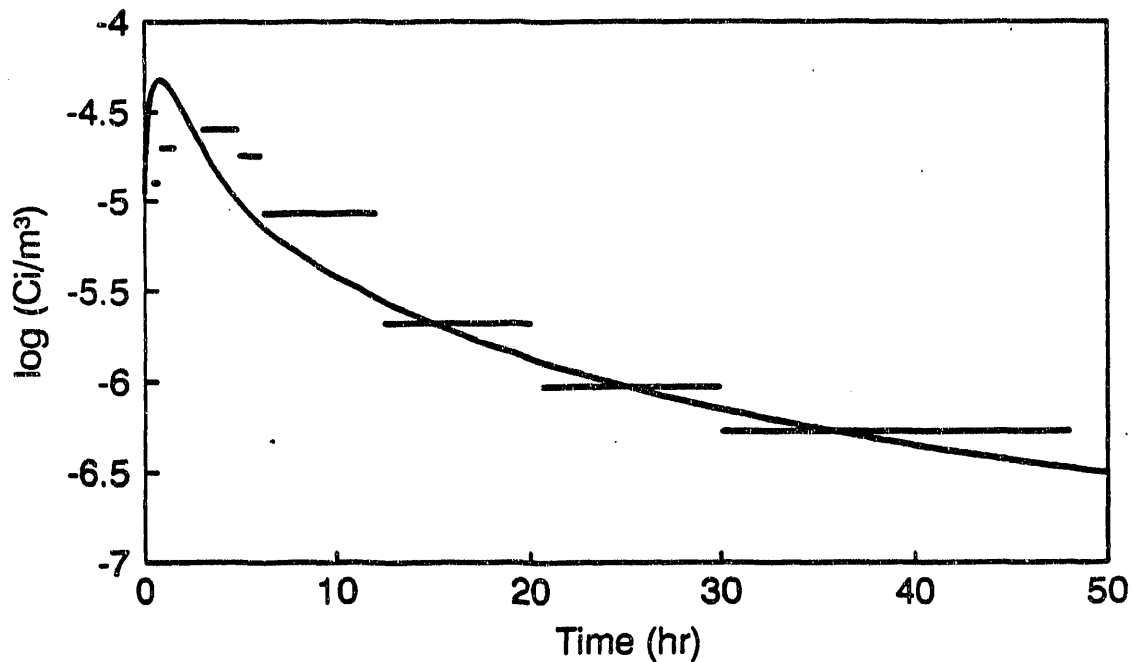
HTO Concentration in TSTA Exposure Chamber

Figure 11. Comparison of TMAP4 calculational result with actual experimental data for the test cell release experiment.

INPUT FILES

Input files are in two groups. One consists of the set of 37 files used in the verification coverage analysis. The second is the set of 14 files used in the validation process. All these files are listed on a diskette available with this report. Only the names of the first group, found in directory "verify" on the diskette are provided here. Files in the validation set are located in directory "valid" on the diskette. They are also listed here for convenience in evaluating the validation problems.

Verification Files

BEO-PROB.INP	3762	03-23-92	7:31p	GEN14.INP	53951	03-05-92	2:55p
CHEM1.INP	1516	03-23-92	10:06p	GEN15.INP	3769	05-14-92	10:57a
CHEM2.INP	1997	03-23-92	10:17p	GEN16.INP	3890	05-14-92	10:58a
CLEANUP.INP	3242	03-23-92	7:31p	GENERAL.INP	17803	08-07-91	12:54p
COMP.INP	3593	12-10-90	10:34a	HE.INP	3343	03-23-92	7:32p
GEN1.INP	51304	03-05-92	2:05p	MOD5-IN.INP	23747	05-14-92	11:07a
GEN1RST.INP	481	05-14-92	12:14p	PROB-1.INP	2381	05-05-92	6:02p
GEN2.INP	47015	03-05-92	2:19p	PROB2CHG.INP	3382	05-19-92	11:45a
GEN3.INP	48607	03-05-92	2:20p	PROB2HT.INP	3660	05-19-92	11:43a
GEN4.INP	52954	03-05-92	2:22p	PROB-3.INP	2446	05-21-92	1:29p
GEN5.INP	52912	03-05-92	2:23p	SH1.INP	1458	05-14-92	11:39a
GEN6.INP	1824	03-05-92	2:37p	SH2.INP	1369	05-14-92	11:41a
GEN7.INP	1821	03-05-92	2:36p	SH3.INP	1301	05-14-92	11:42a
GEN8.INP	1822	03-05-92	2:36p	SH4.INP	1519	05-14-92	11:45a
GEN9.INP	1844	03-05-92	2:37p	SH5.INP	1851	05-14-92	11:45a
GEN10.INP	1846	03-05-92	2:50p	SH6.INP	15865	03-05-92	2:01p
GEN11.INP	1821	03-05-92	2:50p	THERM1.INP	1353	05-14-92	11:46a
GEN12.INP	1814	03-05-92	2:50p	THERM2.INP	1346	05-14-92	11:48a
GEN13.INP	1868	03-05-92	2:51p				

VAL-1A.INP

```
title input
  Validation Problem #1  Tritium diffusion through SiC layer
  with depleting source at 2100 C.  No solubility or trapping included.
end of title input
$
$
main input
  dspcnme=t,end
  espcnme=ts,end
  segnds=9,end
  nbrencl=2,end
end of main input
$
$
enclosure input
  start func,1
  etemp=2373.0,end
  esppres=ts,1.0e6,end
  reaction=nequ,0,end
  evol=5.2e-11,end
$
  start bdry,2
  etemp=2373.0,end
  esppres=ts,0.0,end
end of enclosure input
$
$
thermal input
  start thermseg
  delx=0.0,3.0e-6,6*5.0e-6,0.0,end
  dtemp=9*2373.0,end
end of thermal input
$
$
diffusion input
  start diffseg
  dconc=t,9*0.0,end
  dcoef=t,equ,1,end
  qstrdr=t,equ,3,end
  spcsrc=t,equ,3,srcpf,9*0.0,end
  difbcl=lawdep,encl,1,t,ts,pexp,1.0,solcon,equ,2,end
  difbcr=sconc,encl,2,t,ts,nsurfs,1,conc,const,0.0,end
  surfa=2.16e-6,end
end of diffusion input
$
$
equation input
  y=1.58e-4*exp(-308000.0/(8.314*temp)),end
  y=7.244e22/temp,end
```

```
   y=0.0,end
end of equation input
$
$
table input
end of table input
$
$
control input
   time=0.0,end
   tstep=1.0,end
   timend=140.0,end
   nprint=10,end
   itermx=20000,end
   delcmx=1.0e-7,end
end of control input
$
$
plot input
   nplot=1,end
   plotseg=1,end
   plotencl=1,2,end
   dname=t,end
   ename=ts,end
   dplot=end
   eplot=conc,diff,end
end of plot input
$
end of data
```

```
title input
   Validation Problem #2  -  2100 C -- No solubility or trapping.
   Tritium diffusion through semi-infinite SiC layer w/ constant source.
end of title input
$
$
main input
   dspcnme=t,end
   espcnme=ts,end
   segnds=99,end
   nbrencl=2,end
end of main input
$
$
enclosure input
   start bdry,1
   etemp=2373.0,end
   esppres=ts,1.0e6,end
$
   start bdry,2
   etemp=2373.0,end
   esppres=ts,0.0,end
end of enclosure input
$
$
thermal input
   start thermseg
   delx=0.0,75*0.1,22*10.0,0.0,end
   dtemp=99*2373.0,end
end of thermal input
$
$
diffusion input
   start diffseg
   dconc=t,99*0.0,end
   dcoef=t,equ,1,end
   qstrdr=t,equ,2,end
   spcsrc=t,equ,2,srcpf,99*0.0,end
   difbcl=sconc,encl,1,t,ts,nsurfs,1,conc,const,1.0,end
   difbcr=sconc,encl,2,t,ts,nsurfs,1,conc,const,0.0,end
   surfa=1.0,end
end of diffusion input
$
$
equation input
   y=1.0,end
   y=0.0,end
end of equation input
$
$
table input
end of table input
```

59

```
$
$
control input
   time=0.0,end
   tstep=1.0,end
   timend=50.0,end
   nprint=1,end
   itermx=20000,end
   delcmx=1.0e-7,end
end of control input
$
$
plot input
   nplot=1,end
   plotseg=1,end
   plotencl=1,2,end
   dname=t,end
   ename=ts,end
   dplot=sflux,end
   eplot=end
end of plot input
$
end of data
```

```
title input
   Validation Problem #3  -  Impermeable layer at x=0, t=2100 C.
   Tritium diffusion through semi-infinite partially loaded SiC layer
end of title input
$
$
main input
   dspcnme=td,end
   espcnme=t,end
   segnds=99,end
   nbrencl=1,end
end of main input
$
$
enclosure input
   start bdry,1
   etemp=2373.0,end
   esppres=t,0.0,end
end of enclosure input
$
$
thermal input
   start thermseg
   delx=0.0,75*1.0,22*100.0,0.0,end
   dtemp=99*2373.0,end
end of thermal input
$
$
diffusion input
   start diffseg
   dconc=td,11*1.0,88*0.0,end
   dcoef=td,equ,1,end
   qstrdr=td,equ,2,end
   spcsrc=td,equ,2,srcpf,99*0.0,end
   difbcl=nonflow,end
   difbcr=sconc,encl,1,td,t,nsurfs,1,conc,const,0.0,end
   surfa=1.0,end
end of diffusion input
$
$
equation input
   y=1.0,end
   y=0.0,end
end of equation input
$
$
table input
end of table input
$
$
control input
   time=0.0,end
```

```
      tstep=0.1,end
      timend=101.0,end
      nprint=50,end
      itermx=20000,end
      delcmx=1.0e-7,end
end of control input
$
$
plot input
   nplot=10,end
   plotseg=1,end
   plotencl=1,end
   dname=td,end
   ename=t,end
   dplot=moblinv,sflux,sconc,end
   eplot=diff,end
end of plot input
$
end of data
```

```
title input
  Validation Problem #4a  -  Trapping in a slab of constant upstream
  concentration - effective diffusivity limit
end of title input
$
$
main input
  dspcnme=td,end
  espcnme=t,end
  segnds=22,end
  nbrencl=2,end
end of main input
$
$
enclosure input
  start bdry,1
  etemp=1000.0,end
  esppres=t,1.0,end
$
  start bdry,2
  etemp=1000.0,end
  esppres,t,0.0,end
end of enclosure input
$
$
thermal input
  start thermseg
  delx=0.0,20*0.05,0.0,end
  dtemp=22*1000.0,end
end of thermal input
$
$
diffusion input
  start diffseg
  dconc=td,22*0.0,end
  dcoef=td,equ,1,end
  ctrap=td,22*0.0,end
  qstrdr=td,equ,2,end
  trapping=cetrpi,0.1,nbrden,3.1622e22,td,alpht,equ,3,alphr,equ,4,end
  spcsrc=td,equ,2,srcpf,22*0.0,end
  difbcl=sconc,encl,1,td,t,nsurfs,1,conc,const,3.1622e18,end
  difbcr=sconc,encl,2,td,t,nsurfs,1,conc,const,0.0,end
  surfa=1.0,end
end of diffusion input
$
$
equation input
  y=1.0,end
  y=0.0,end
  y=1.0e15,end
  y=1.0e13*exp(-100./temp),end
end of equation input
```

```
$
$
table input
end of table input
$
$
control input
   time=0.0,end
   tstep=0.01,end
   timend=3.0,end
   nprint=60,end
   itermx=200,end
   delcmx=1.0e-5,end
end of control input
$
$
plot input
   nplot=1,end
   plotseg=1,end
   plotencl=end
   dname=td,end
   ename=end
   dplot=sflux,end
   eplot=end
end of plot input
$
end of data
```

```
title input
  Validation Problem #4b  -   Trapping in a slab of constant upstream
  concentration - strong-trapping limit
end of title input
$
$
main input
  dspcnme=td,end
  espcnme=t,end
  segnds=22,end
  nbrencl=2,end
end of main input
$
$
enclosure input
  start bdry,1
  etemp=1000.0,end
  esppres=t,1.0,end
$
  start bdry,2
  etemp=1000.0,end
  esppres,t,0.0,end
end of enclosure input
$
$
thermal input
  start thermseg
  delx=0.0,20*0.05,0.0,end
  dtemp=22*1000.0,end
end of thermal input
$
$
diffusion input
  start diffseg
  dconc=td,22*0.0,end
  dcoef=td,equ,1,end
  ctrap=td,22*0.0,end
  qstrdr=td,equ,2,end
  trapping=cetrpi,0.1,nbrden,3.1622e22,td,alpht,equ,3,alphr,equ,4,end
  spcsrc=td,equ,2,srcpf,22*0.0,end
  difbcl=sconc,encl,1,td,t,nsurfs,1,conc,const,3.1622e18,end
  difbcr=sconc,encl,2,td,t,nsurfs,1,conc,const,0.0,end
  surfa=1.0,end
end of diffusion input
$
$
equation input
  y=1.0,end
  y=0.0,end
  y=1.0e15,end
  y=1.0e13*exp(-10000./temp),end
end of equation input
```

65

```
$
$
table input
end of table input
$
$
control input
  time=0.0,end
  tstep=2.0,end
  timend=1000.0,end
  nprint=50,end
  itermx=200,end
  delcmx=1.0e-4,end
end of control input
$
$
plot input
  nplot=1,end
  plotseg=1,end
  plotencl=end
  dname=td,end
  ename=end
  dplot=sflux,end
  eplot=end
end of plot input
$
end of data
```

```
title input
  Validation Problem #5  -   Tritium diffusion through PyC/SiC layer in NPR
  fuel particles at 2100 C with constant source and no solubility.
end of title input
$
$
main input
  dspcnme=td,end
  espcnme=t,end
  segnds=9,9,end
  nbrencl=2,end
  linksegs=1,2,end
end of main input
$
$
enclosure input
  start bdry,1
  etemp=2373.0,end
  esppres=t,1.0e6,end
$
  start bdry,2
  etemp=2373.0,end
  esppres,t,0.0,end
end of enclosure input
$
$
thermal input
  start thermseg
  delx=0.0,3.0e-6,6*1.0e-5,0.0,end
  dtemp=9*2373.0,end
$
  start thermseg
  delx=0.0,3.0e-6,5.0e-6,0.0,4*6.25e-6,0.0,end
  dtemp=9*2373.0,end
end of thermal input
$
$
diffusion input
  start diffseg
  dconc=td,9*0.0,end
  dcoef=td,equ,1,end
  qstrdr=td,equ,3,end
  spcsrc=td,equ,3,srcpf,9*0.0,end
  difbcl=sconc,encl,1,td,t,nsurfs,1,conc,const,3.0537e25,end
  difbcr=link,td,solcon,equ,4,end
  surfa=2.16e-6,end
$
  start diffseg
  dconc=td,9*0.0,end
  dcoef=td,equ,2,end
  qstrdr=td,equ,3,end
  spcsrc=td,equ,3,srcpf,9*0.0,end
```

67

```
   difbcr=sconc,encl,2,td,t,nsurfs,1,conc,const,0.0,end
   difbcl=link,td,solcon,equ,4,end
   surfa=2.16e-6,end
end of diffusion input
$
$
equation input
   y=1.0e-1*exp(-64000.0/(1.987*temp)),end
   y=1.58e-4*exp(-308000.0/(8.314*temp)),end
   y=0.0,end
   y=1.0,end
end of equation input
$
$
table input
end of table input
$
$
control input
   time=0.0,end
   tstep=1.0,end
   timend=200.0,end
   nprint=5,end
   itermx=20000,end
   delcmx=1.0e-6,end
end of control input
$
$
plot input
   nplot=1,end
   plotseg=1,end
   plotencl=1,2,end
   dname=td,end
   ename=t,end
   dplot=moblinv,end
   eplot=diff,end
end of plot input
$
end of data
```

68

```
title input
   Validation Problem #6a   -   Model Utilizes TMAP4 Thermal Capabilities
   Heat Conduction in Slab with Internal Heat Generation
end of title input
$
$
main input
   dspcnme=qd,end
   espcnme=q,end
   segnds=10,end
   nbrencl=1,end
end of main input
$
$
enclosure input
   start bdry,1
   etemp=300.0,end
   esppres=q,0.0,end
end of enclosure input
$
$
thermal input
   start thermseg
   delx=0.0,8*0.20,0.0,end
   dtemp=10*1000.0,end
   tcon=const,10.0,end
   rhocp=const,1.0,end
   hsrc=const,1.0e4,srcpf,10*1.0,end
   htrbcl=adiab,end
   htrbcr=stemp,const,300.0,end
end of thermal input
$
$
diffusion input
   start diffseg
   dconc=qd,10*0.0,end
   dcoef=qd,const,0.1,end
   qstrdr=qd,const,0.0,end
   spcsrc=qd,const,0.0,srcpf,10*0.0,end
   difbcl=nonflow,end
   difbcr=sconc,encl,1,qd,q,nsurfs,1,conc,const,0.0,end
   surfa=1.0,end
end of diffusion input
$
$
equation input
end of equation input
$
$
table input
end of table input
$
```

```
$
control input
   time=0.0,end
   tstep=1.0,end
   timend=50.0,end
   nprint=5,end
   itermx=200,end
   delcmx=1.0e-6,end
end of control input
$
$
plot input
   nplot=5,end
   plotseg=1,end
   plotencl=1,end
   dname=qd,end
   ename=q,end
   dplot=end
   eplot=end
end of plot input
$
end of data
```

```
title input
   Validation Problem #6b  -  Model Utilizes TMAP4 Thermal Capabilities
   Prediction of Slab Temperature as a function of Time
end of title input
$
$
main input
   dspcnme=td,end
   espcnme=t,end
   segnds=18,end
   nbrencl=1,end
end of main input
$
$
enclosure input
   start bdry,1
   etemp=373.0,end
   esppres=t,0.0,end
end of enclosure input
$
$
thermal input
   start thermseg
   delx=0.0,1.25e-2,14*2.5e-2,1.25e-2,0.0,end
   dtemp=18*300.0,end
end of thermal input
$
$
diffusion input
   start diffseg
   dconc=td,18*300.0,end
   dcoef=td,const,1.29035e-3,end
   qstrdr=td,const,0.0,end
   spcsrc=td,const,0.0,srcpf,18*0.0,end
   difbcl=nonflow,end
   difbcr=sconc,encl,1,td,t,nsurfs,1,conc,const,373.0,end
   surfa=1.0,end
end of diffusion input
$
$
equation input
end of equation input
$
$
table input
end of table input
$
$
control input
   time=0.0,end
   tstep=10.0,end
   timend=180.0,end
```

```
     nprint=6,end
     itermx=2000,end
     delcmx=1.0e-6,end
end of control input
$
$
plot input
    nplot=1,end
    plotseg=1,end
    plotencl=end
    dname=td,end
    ename=end
    dplot=sconc,end
    eplot=end
end of plot input
$
end of data
```

```
title input
   Validation Problem #7a  -  Simple Chemical Reaction Problem
       Equal Starting Concentrations
end of title input
$
$
main input
  dspcnme=q,end
  espcnme=a,b,ab,end
  segnds=3,end
  nbrencl=1,end
end of main input
$
$
enclosure input
   start func,1
   etemp=300.0,end
   esppres=a,1.0e-6,b,1.0e-6,ab,0.0,end
   reaction=nequ,1
      ratequ,1,nreact,2,a,1.0,b,1.0,nprod,1,ab,1.0,end
   evol=10.0,end
end of enclosure input
$
$
thermal input
   start thermseg
   delx=0.0,1.0,0.0,end
   dtemp=3*300.0,end
end of thermal input
$
$
diffusion input
   start diffseg
   dconc=q,3*0.0,end
   dcoef=q,const,1.0,end
   qstrdr=q,const,0.0,end
   spcsrc=q,const,0.0,srcpf,3*0.0,end
   difbcl=nonflow,end
   difbcr=nonflow,end
   surfa=1.0,end
end of diffusion input
$
$
equation input
  y=4.14e-15*conc(1)*conc(2),end
end of equation input
$
$
table input
end of table input
$
$
```

```
control input
  time=0.0,end
  tstep=0.01,end
  timend=50.1,end
  nprint=1000,end
  itermx=200,end
  delcmx=1.0e-6,end
end of control input
$
$
plot input
  nplot=100,end
  plotseg=end
  plotencl=1,end
  dname=end
  ename=a,b,ab,end
  dplot=end
  eplot=conc,end
end of plot input
$
end of data
```

```
title input
   Validation Problem #7b  -  Simple Chemical Reaction Problem
       Unequal Starting Concentrations
end of title input
$
$
main input
   dspcnme=q,end
   espcnme=a,b,ab,end
   segnds=3,end
   nbrencl=1,end
end of main input
$
$
enclosure input
   start func,1
   etemp=300.0,end
   esppres=a,1.0e-6,b,1.0e-7,ab,0.0,end
   reaction=nequ,1
      ratequ,1,nreact,2,a,1.0,b,1.0,nprod,1,ab,1.0,end
   evol=10.0,end
end of enclosure input
$
$
thermal input
   start thermseg
   delx=0.0,1.0,0.0,end
   dtemp=3*300.0,end
end of thermal input
$
$
diffusion input
   start diffseg
   dconc=q,3*0.0,end
   dcoef=q,const,1.0,end
   qstrdr=q,const,0.0,end
   spcsrc=q,const,0.0,srcpf,3*0.0,end
   difbcl=nonflow,end
   difbcr=nonflow,end
   surfa=1.0,end
end of diffusion input
$
$
equation input
   y=4.14e-15*conc(1)*conc(2),end
end of equation input
$
$
table input
end of table input
$
$
```

```
control input
   time=0.0,end
   tstep=0.01,end
   timend=50.1,end
   nprint=1000,end
   itermx=200,end
   delcmx=1.0e-6,end
end of control input
$
$
plot input
   nplot=100,end
   plotseg=end
   plotencl=1,end
   dname=end
   ename=a,b,ab,end
   dplot=end
   eplot=conc,end
end of plot input
$
end of data
```

```
title input
   TMAP Validation Problem #8 - System (Multiple Enclosure Volumes) Problem
end of title input
$
main input
   dspcnme=t,end
   espcnme=t2,end
     segnds =3,end
     nbrencl=3,end
end of main input
$
enclosure input
$
start func,2
   etemp=303.,end
   esppres = t2,0.0,end
   reaction = nequ,0,end
   evol = 1.0,end
   outflow = nbrflwp,1,qflow,const,0.1,rencl,3,end
start func,3
   etemp=303.,end
   esppres = t2,0.0,end
   reaction = nequ,0,end
   evol = 1.0,end
   outflow = nbrflwp,1,qflow,const,0.1,rencl,1,end
start bdry,1
   etemp = 303.,end
   esppres = t2,const,1.0,end
   outflow = nbrflwp,1,qflow,const,0.1,rencl,2,end
end of enclosure input
$
thermal input
$
start thermseg
   delx=0.0,1.0,0.0,end
   dtemp=3*303.0,end
end of thermal input
$
diffusion input
start diffseg
   dconc=t,3*0.0,end
   dcoef=t,const,1.0,end
   qstrdr=t,const,0.0,end
   spcsrc=t,const,0.0,srcpf,3*0.0,end
   difbcl=nonflow,end
   difbcr=nonflow,end
   surfa=1.0,end
end of diffusion input
$
equation input
end of equation input
$
```

```
table input
end of table input
$
control input
 time=0.0,end
 tstep=0.01,end
 timend=20.0,end
 nprint=50,end
 itermx=20,end
 delcmx=1.e-6,end
end of control input
$
plot input
 nplot=100,end
 plotseg=end
 plotencl=2,3,end
 dname=end
 ename=t2,end
 dplot=end
 eplot=conc,conv,end
end of plot input
$
end of data
```

```
title input
SAMPLE PROBLEM No.1 - Plasma driven permeation of PCA
end of title input
$
main input
   dspcnme=d,end
   espcnme=d2,end
   segnds=21,end
   nbrencl=2,end
end of main input
$
enclosure input
$
start bdry,1,end                                    $Implantation side
   etemp=703.,end
   esppres=d2,tabl,1,end
start bdry,2,end                                    $Downstream side
   etemp=703.,end
   esppres=d2,const,2.e-6,end
end of enclosure input
$
thermal input
start thermseg,end
   delx=0.0,5*4.0e-9,1.0e-8,1.0e-7,1.0e-6,1.0e-5,10*4.88e-5,0.0,end
   dtemp=21*703.,end
end of thermal input
$
diffusion input
start diffseg,end
   dconc=d,21*0.0,end
   dcoef=d,const,3.0e-10,end                        $Diffusivity (m2/s)
   qstrdr=d,const,0.0,end                           $No temperature gradient
   spcsrc=d,tabl,2,srcpf,3*0.0,0.25,1.0,0.25,15*0.0,end
   difbcl=ratedep,encl,1,d
          d2,ksubd,equ,1,d,ksubr,equ,2,end
   difbcr=ratedep,encl,2,d
          d2,ksubd,const,1.7918e15,d,ksubr,const,2.0e-31,end
     surfa=1.0,end                                  $Answers will be d/m^2
end of diffusion input
$
equation input
$ Dissociation constant (d_2/m^2.s.Pa^1/2)
  y = 8.959e18*(1.0-0.9999*exp(-6.0e-5*time)),end $Eq.1
$ Recombination constant (m^4/d_2.s)
  y = 1.0e-27*(1.0-0.9999*exp(-6.0e-5*time)),end $Eq.2
end of equation input
$
table input
$ Upstream enclosure pressure history
  0.0,4.0e-5,6420.0,4.0e-5,6420.1,9.0e-6,9420.0,9.0e-6,9420.1,4.0e-5
  12480.0,4.0e-5,12480.1,9.0e-6,14940.0,1.9e-6,14940.1,4.0e-5,18180.0
  4.0e-5,18180.1,9.0e-6,1.0e10,9.0e-6,end           $Table 1
```

```
$ Implantation flux (d/m2s)
 0.0,4.9e19,6420.0,4.9e19,6420.1,0.0,9420.0,0.0,9420.1,4.9e19
 12480.0,4.9e19,12480.1,0.0,14940.0,0.0,14940.1,4.9e19,18180.0
 4.9e19,18180.1,0.0,1.0e10,0.0,end                      $Table 2
end of table input
$
control input
 time=0.0,end
 tstep=20.0,end                                     $ Seconds
 timend=19200.,end                                  $ 320 minutes for problem
 nprint=60,end                                      $ Print out every 20 min
 itermx=90,end
 delcmx=1.e-8,end
end of control input
$
plot input
 nplot=3,end                                        $ Plot points every minute
 plotseg=1,end
 plotencl=1,2,end
 dname=d,end
 ename=d2,end
 dplot=moblinv,sflux,end
 eplot=end
end of plot input
end of data
```

```
title input
R. G. Macaulay-Newcombe's thermal charging problem for gas absorption into
     a wafer of polished beryllium with a thin oxide film.
end of title input
$
main input
  dspcnme=d,end
  espcnme=d2,end
  segnds =20,17,end                              $ Oxide has 20, Be has 17
  nbrencl=1,end
  linksegs=1,2,end                               $ The oxide and Be are joined
end of main input
$
enclosure input
$
start bdry,1,end                                 $ Outside of sample
  etemp=773.00,end
  esppres=d2,equ,6,end                           $ Pressure history in Eq.6
end of enclosure input
$
thermal input
$ Segment 1 - BeO film
start thermseg,end
   delx=0.0,18*1.0e-9,0.0,end
   dtemp=20*773.0,end
   tcon=const,159.2,end
   rhocp=const,3.0e6,end
   hsrc=const,0.0,srcpf,20*0.0,end
   htrbcl=stemp,equ,1,end                        $ Temperature history in Eq.1
   htrbcr=link,end
   hgap=const,1.e6,end
$ Segment 2 - Be metal - half thick
start thermseg,end
   delx=0.0,1.0e-9,1.e-8,1.e-7,1.e-6,1.e-5,10*1.888e-5,0.0,end
   dtemp=17*773.0,end
   tcon=const,168.0,end
   rhocp=const,3.37e6,end
   hsrc=const,0.0,srcpf,17*0.0,end
   htrbcl=link,end
   htrbcr=adiab,end
end of thermal input
$
diffusion input
$ Seg No. 1  BeO film
start diffseg,end
  dconc=d,20*0.0,end
  dcoef=d,equ,2,end                              $ D for d in BeO in Eq.2
  qstrdr=d,const,0.0,end                         $ Q* of no consequence
  spcsrc=d,const,0.0,srcpf,20*0.0,end
  difbcl=lawdep,encl,1
            d
          d2,pexp,0.5,solcon,equ,3,end
```

```
    difbcr=link,d,solcon,equ,3,end                    $ Solubility for D in BeO in
Eq.3
    surfa=1.04e-4,end
$ Seg No. 2   Be foil - half thickness
start diffseg,end
    dconc=d,17*0.0,end
    dcoef=d,equ,4,end                                 $ D for d in Be in Eq.4
    qstrdr=d,const,0.0,end                            $ Q* of no consequence
    spcsrc=d,const,0.0,srcpf,17*0.0,end
    difbcl=link,d,solcon,equ,5,end                    $ Solubility for D in Be in
Eq.5
    difbcr=nonflow,end                                $ Midplane of foil - no flow
    surfa=1.04e-4,end
end of diffusion input
$
equation input
$ Temperature history equation
  y = 773.-int(time/180000.)*(1-exp(-(time-180000.)/2700.))*475.,end $Eq.1 Temp
$ Diffusion and solubility equations
  y = 1.40e-4*exp(-24408./temp),end                   $Eq.2 D of d in BeO (Fowler 1)
  y = 5.00e20*exp(9377.7/temp),end                    $Eq.3 S for d in BeO
  y = 8.0e-9*exp(-4220./temp),end                     $Eq.4 D of d in Be (Abramov
Be-2).
  y = 7.156e27*exp(-11606./temp),end                  $Eq.5 S for d in Be (Swansiger)
$ Pressure history equation
      13300.0*(1-int(time/180015.))+1.0e-6,end·       $Eq.6 Pressure history
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end                                        $ Seconds
  tstep=60.0,end                                      $ One minute time step
  timend=182400.,end                                  $ 50 hr + 45 min cooling
  nprint=300,end                                      $ Output at 5-hr intervals
  itermx=90,end
  delcmx=1.e-8,end
end of control input
$
plot input
  nplot=10,end                                        $ Cycles
  plotseg=1,2,end
  plotencl=end
  dname=d,end
  ename=end
  dplot=moblinv,sflux,end
  eplot=end
end of plot input
end of data
```

```
restart
$
equation input
$ Temperature history equation
 y = 300.0+0.05*time,end                      $Eq.1 Heat rate 3 K/min

$ Diffusion and solubility equations
 y = 7.00e-5*exp(-27000./temp),end            $Eq.2 D of d in BeO (Fowler 2)
 y = 5.00e20*exp(9377.7/temp),end             $Eq.3 S for d in BeO
 y = 8.0e-9*exp(-4220./temp),end              $Eq.4 D of d in Be (Abramov
Be-2)
 y = 7.156e27*exp(-11606./temp),end           $Eq.5 S for d in Be (Swansiger)
$ Pressure history equation
 y = 0.001,end                                $Eq.6 Pressure history
end of equation input
$
table input
end of table input
$
control input
 time=0.0,end
 tstep=60.0,end                               $ One minute sampling
 timend=15460.,end                            $ Time to 800 C
 nprint=10,end                                $ Cycles
 itermx=90,end
 delcmx=1.e-8,end
end of control input
end of data
```

```
title input
  SAMPLE PROBLEM 3 - HTO history in an exposure chamber at TSTA
end of title input
$
main input
  dspcnme=t2d,htd,htod,h2od,end
  espcnme=t2,ht,hto,h2o,end
  segnds=12,end
  nbrencl=3,end
end of main input
$
enclosure input
start func,2,end                $ Tritium exposure chamber
  etemp=303.,end
  esppres=t2,0.434,ht,0.,hto,0.,h2o,714.,end
  outflow=nbrflwp,1,qflow,const,1.5e-4,rencl,3,end
  reaction=nequ,2,ratequ,1
            nreact,2,t2,1.,h2o,1.,nprod,2,hto,1.,ht,1.
                ratequ,2
            nreact,2,ht,1.,h2o,1.,nprod,1,hto,1.,end
  evol=0.96,end
start bdry,1,end                $ Source air from room
  etemp=303.,end
  esppres=t2,0.,ht,0.,hto,0.,h2o,714.,end
  outflow=nbrflwp,1,qflow,const,1.5e-5,rencl,2,end  $Low by 10 x
start bdry,3,end                $ Sink, TWT system
  etemp=303.,end
  esppres=t2,0.,ht,0.,hto,0.,h2o,714.,end
end of enclosure input
$
thermal input
start thermseg                  $ Paint inside the exposure chamber
  delx=0.,10*1.6e-5,0.,end
  dtemp=12*303.,end
end of thermal input
$
diffusion input
start diffseg
  dconc=t2d,12*0.,htd,12*0.,htod,12*0.,h2od,12*0.,end
  dcoef=t2d,const,4.e-12,htd,const,4.e-12
        htod,const,1.e-14,h2od,const,1.e-14,end
  qstrdr=t2d,const,0.,htd,const,0.,htod,const,0.,h2od,const,0. end
  spcsrc=t2d,const,0.,srcpf,12*0.,htd,const,0.,srcpf,12*0.
        htod,const,0.,srcpf,12*0.,h2od,const,0.,srcpf,12*0.,end
  difbcl=lawdep,encl,2,t2d,t2,pexp,1.,solcon,const,4.e19
                  htd,ht,pexp,1.,solcon,const,4.e19
                htod,hto,pexp,1.,solcon,const,6.e19
                h2od,h2o,pexp,1.,solcon,const,6.e24,end
  difbcr=nonflow,end
  surfa=5.6,end
end of diffusion input
$
```

```
equation input
$ Reaction rate equations
$    Index for conc array is relative enclosure specie number
$        (i.e., t2=1, ht=2, hto=3, h2o=4)
  y = 2.0e-29*conc(1)*(2.*conc(1)+conc(2)+conc(3)),end  $ Eq.1
  y = 1.0e-29*conc(2)*(2.*conc(1)+conc(2)+conc(3)),end  $ Eq.2
end of equation input
$
table input
end of table input
$
control input
  time=0.,end
  tstep=60.,end
  timend=180000.,end
  nprint=600,end
  itermx=90,end
  delcmx=1.e-5,end
end of control input
$
plot input
  nplot=5,end
  plotseg=1,end
  plotencl=2,3,end
  dname=t2d,htd,htod,htod,end
  ename=t2,ht,hto,end
  dplot=moblinv,sflux,end
  eplot=conc,end
end of plot input
end of data
```

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