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Verification and Validation of TMAP7

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Bechtel BWXT Idaho, LLC

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ABSTRACT

The Tritium Migration Analysis Program, Version 7 (TMAP7) code is an update of TMAP4, an earlier version that was verified and validated in support of the International Thermonuclear Experimental Reactor (ITER) program and of the intermediate version TMAP2000. It has undergone several revisions. The current one includes radioactive decay, multiple trap capability, more realistic treatment of heteronuclear molecular formation at surfaces, processes that involve surface-only species, and a number of other improvements. Prior to code utilization, it needed to be verified and validated to ensure that the code is performing as it was intended and that its predictions are consistent with physical reality. To that end, the demonstration and comparison problems cited here show that the code results agree with analytical solutions for select problems where analytical solutions are straightforward or with results from other verified and validated codes, and that actual experimental results can be accurately replicated using reasonable models with this code. These results and their documentation in this report are necessary steps in the qualification of TMAP7 for its intended service.

This revision corrects minor inconsistencies in the previous version and reflects results from the 2008 revision of the TMAP7 code. It also includes some additional demonstration problems.

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1.0 OVERVIEW

The TMAP Code was written at the Idaho National Engineering and Environmental Laboratory by Brad Merrill and James Jones in the late 1980s as a tool for safety analysis of systems involving tritium. [1]Since then it has been upgraded to TMAP4 and has been used in numerous applications including experiments supporting fusion safety, predictions for advanced systems such as the International Thermonuclear Experimental Reactor (ITER), and estimates involving tritium production technologies. The code's further upgrade to TMAP2000[2] and now to TMAP7 was accomplished in response to several needs. TMAP and TMAP4 had the capacity to deal with only a single trap for diffusing gaseous species in solid structures. TMAP7 includes up to three separate traps and up to 10 diffusing species. The difficulty dealing with heteronuclear molecule formation such as HD under solution-law dependent diffusion boundary conditions, such as Sieverts' law, has been corrected. TMAP7 automatically generates heteronuclear molecular partial pressures and surface flows when solubilities and partial pressures of the homonuclear molecular species are provided. A further sophistication is the addition of non-diffusing surface species. Atoms such as oxygen or nitrogen or complexes such as hydroxyl radicals on metal surfaces are sometimes important in molecule formation with diffusing hydrogen isotopes but do not themselves diffuse appreciably in the material. TMAP7 will accommodate up to 30 such surface species, allowing the user to specify relationships between those surface concentrations and partial pressures of gaseous species above the surfaces or to form them dynamically by combining diffusion species or other surface species. Additionally, TMAP7 allows the user to include a surface binding energy and an adsorption barrier energy and includes asymmetrical diffusion between the surface sites and regular diffusion sites in the bulk. All of the previously existing features for heat transfer, flows between enclosures, and chemical reactions within the enclosures have been retained, but the allowed problem size and complexity have been increased to take advantage of the greater memory and speed available on modern computers. One feature unique to TMAP7 is the addition of radioactive decay for both trapped and mobile species. Another is the ability to initialize distributed parameters such as initial mobile atom, trapped atom, or trap concentrations using selected mathematical functions. Also, time-dependent temperatures and pressures can be specified in *boundary* enclosures and for surface concentrations of diffusion species.

The verification and validation process normally involves two steps. In the verification process, a careful examination of the code ensured that the coding faithfully reproduces the mathematical model and that the code is well written and efficient. That process was pursued extensively with TMAP4. Independent verification has not been done independently of code development for TMAP7. The basic architecture of the code remains the same, although a number of changes were required to work with the GNU FORTRAN 77, selected for distribution with the code. There are also new components and a few new subroutines. These have been carefully evaluated for coding accuracy, but the demonstration of their success is in the high fidelity the code provides to the sample problems. Those sample problems constitute the validation of the code and provide the basis for what is presented here.

There are two main sections to this report. The first exercises TMAP7 in each of its major capability areas using specialized problems, showing that the results computed by TMAP7 are in good agreement with “known” results. This demonstrates that the code's functional tools are performing properly. The second part of the report provides a comparison of TMAP7 results with experimental results to show the general utility of the code in modeling reality.

2.0 SPECIALIZED PROBLEMS

Computational capabilities of TMAP7 lie in six major areas: diffusion and trapping within structures and surface processes, heat transfer, chemical reactions in enclosures, bulk fluid flows, chemical equilibrium and radioactive decay. The demonstration problems that follow are grouped into those areas.

Problems 1a-1e exercise TMAP7's mass transfer capabilities

Problems 1f (a-d) demonstrate TMAP7's heat transfer functions

Problems 1g (a-c) model enclosure reactions

Problems 1h (a-b) deal with enclosure flow

Problem 1i (a-d) verify chemical reactions in enclosures and on surfaces are correct

Problem 1j (a-b) demonstrate radioactive decay.

The descriptions of these problems include a statement of the problem, a description of the modeling used in setting up the problem for TMAP7, and a comparison of the TMAP7 results with "known" solutions from literature or other sources. Appendix A is the derivation for the surface equilibrium model used in problem 1i (b). Appendix B contains the input code listings for each of the problems cited in the report.

The file names assigned to the various problems appear in parentheses in the headings for the problem descriptions. Input files carry the *.inp* extension, output or *codeout* files have *.out* extensions, and plot data files (*pltdata*) terminate with the *.plt* extension.

Theoretical results were calculated using Microsoft Excel™, and TMAP7 calculations were obtained in two working environments. One used Windows XP™ on a Dell Optiplex GX 260 and again on a Dell Optiplex GX-620. The other was Windows ME™ running on a Dell Dimension XPS R450 and on a Dell Latitude 600 laptop computer.

2.1 Problem 1a: Diffusion from a Depleting Source (Val-1a)

This diffusion problem models an enclosure that is pre-charged with a fixed quantity of tritium. At time $t > 0$, the tritium is allowed to diffuse through a finite slab of SiC, initially at zero concentration. The surface of the slab in contact with the source is assumed to be in equilibrium with the source enclosure. The boundary condition at the exit side of the slab is kept constant at zero concentration for all time. The concentration of the enclosure is then calculated for different times and reported as a fractional release. There are no trapping effects active in the slab.

Carslaw and Jaeger[3] give the analytical solution for an analogous heat transfer problem from which the solute concentration profile in the membrane is

$$C(x,t) = 2SP_0 L \sum_{n=1}^{\infty} \frac{\exp\left(-\alpha_n^2 Dt\right)\sin(\alpha_n x)}{\left[l\left(\alpha_n^2 + L^2\right) + L\right]\sin\left(\alpha_n l\right)} \tag{1}$$

where

$$\alpha_n = \frac{L}{\tan(\alpha_n l)} \tag{2}$$

$$L = \frac{STAk}{V} \tag{3}$$

Here

A = cross-sectional area of the slab (2.16×10^{-6} m^2)

D = diffusivity of tritium (SiC assumed: 2.6237E-11 m^2/s at 2373 K)

k = Boltzmann's constant (1.38065×10^{-23} J/K)

l = thickness of the slab (3.30×10^{-5} m)

S = solubility of tritium (SiC assumed: 3.053×10^{29} kg m^2/s^2)

T = temperature (2373 K)

V = volume of the enclosure (5.20×10^{-11} m^3)

We apply Henry's law to the concentration at $x = l$ to find the gas pressure in the enclosure

$$P(t) = \frac{C(l,t)}{S} = 2P_0 L \sum_{n=1}^{\infty} \frac{\exp\left(-\alpha_n^2 Dt\right)}{l\left(\alpha_n^2 + L^2\right) + L} \tag{4}$$

and finally the release fraction

$$FR = \frac{P(t)}{P_0} = 2L \sum_{n=1}^{\infty} \frac{\exp\left(-\alpha_n^2 Dt\right)}{l\left(\alpha_n^2 + L^2\right) + L} \tag{5}$$

Some of the values obtained from Equation (5) and from TMAP7 are compared in Table 1. Ten terms were included in the sum of Equation (5) so that even at t = 1 s, the last term was less than 10^{-10} of the sum. The variance between the analytical solution and the computed solution from TMAP7 is defined by Equation (6).

$$Variance = \frac{TMAP7 - Analytical}{Analytical} \tag{6}$$

Table 1. Fractional release of tritium from depleting source problem Val-1a.

Time	TMAP7	Theory	Variance
0	0	0	0
1	0.166589	0.201078	-0.171524
2	0.242353	0.265929	-0.088655
3	0.291929	0.310049	-0.058444
4	0.329235	0.343941	-0.042757
5	0.359272	0.371571	-0.033099

Time	TMAP7	Theory	Variance
6	0.384472	0.394945	-0.026516
7	0.406246	0.415252	-0.021687
8	0.425494	0.433273	-0.017954
9	0.442803	0.449553	-0.015015
10	0.458606	0.464482	-0.012651
11	0.473206	0.478348	-0.010751
12	0.486829	0.491366	-0.009233
13	0.499665	0.503693	-0.007997
14	0.511834	0.51545	-0.007015
15	0.523442	0.526726	-0.006234
16	0.534565	0.537588	-0.005623
17	0.545273	0.548089	-0.005139
18	0.555615	0.558269	-0.004754
19	0.565623	0.568157	-0.004459
20	0.575329	0.577778	-0.004238
21	0.584764	0.58715	-0.004063
22	0.593948	0.596289	-0.003926
23	0.602891	0.605206	-0.003825
24	0.611609	0.613913	-0.003753
25	0.620118	0.622417	-0.003693

The variance decreases almost monotonically for $t > 25$ s. Figure 1 shows the comparison for the first 140 s.

A further comparison may be made by noting that the surface flux at $x = 0$ is

$$J = D\frac{\partial C(x,t)}{\partial x}\bigg|_{x=0} = 2SP_0LD\sum_{n=1}^{\infty}\frac{\exp\left(-\alpha_n^2 Dt\right)\alpha_n}{\left[l\left(\alpha_n^2 + L^2\right) + L\right]\sin\left(\alpha_n l\right)} \tag{7}$$

A comparison of results for flux through the free surface is shown in Figure 2.

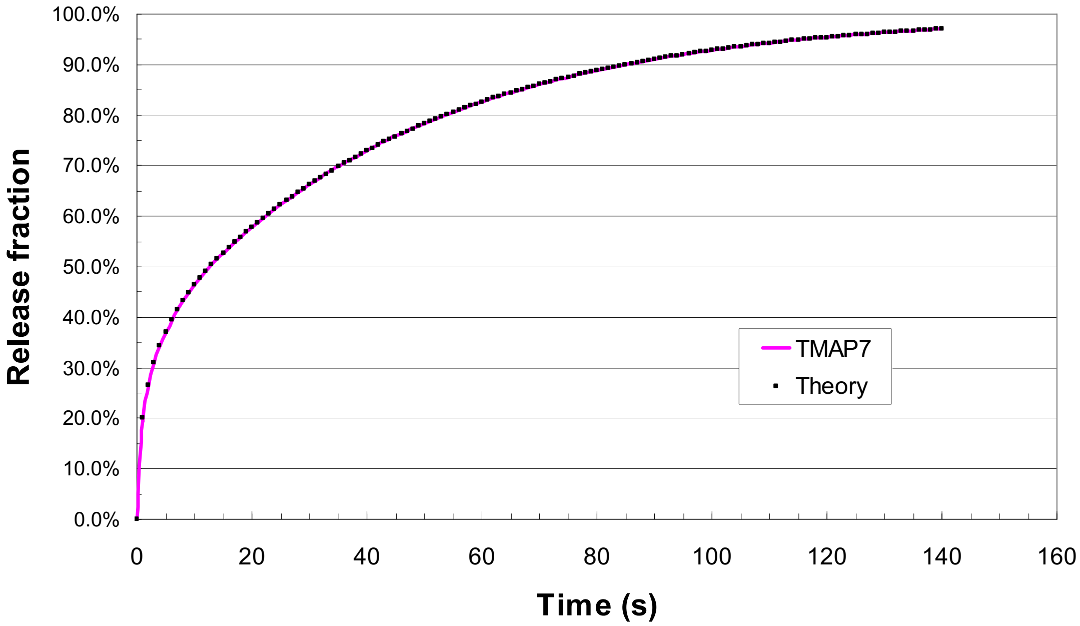

Figure 1. Fractional release of tritium from an enclosure through SiC in depleting source demonstration problem (Val-1a).

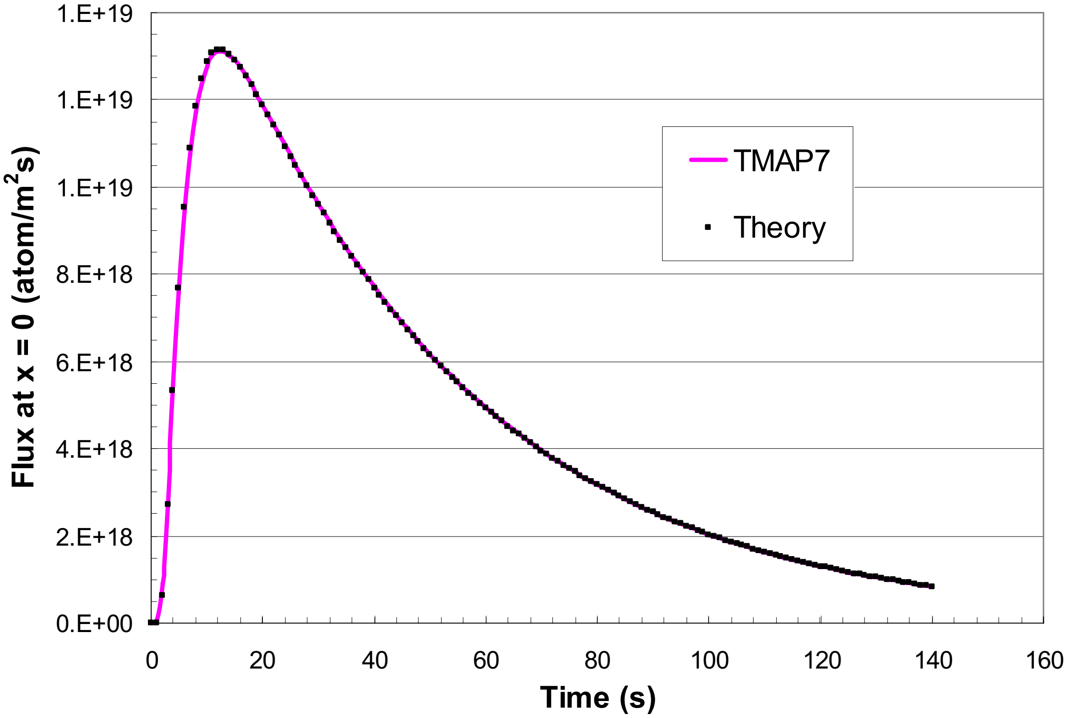

Figure 2. Atom flux through outside face of membrane for depleting source problem (Val-1a).

2.2 Problem 1b: Diffusion in a Semi-Infinite Slab with Constant-Source Boundary (Val-1b)

This model is designed to test the basic Fick's-law diffusion. A semi-infinite slab is defined with a constant concentration boundary condition. The initial concentration of the slab is zero for time, $t \leq 0$ *seconds*. At time $t > 0$, the diffusion is allowed to proceed. The slab is assumed to have no traps. Three comparisons are shown; a transient concentration history at a given location, a spatial concentration profile at a given time, and the variation of flux into the slab surface. These are compared with analytical results.

Carslaw and Jaeger[4] give the analytical solution to the time-dependent concentration profile as

$$C(x,t) = C_o erfc\left(\frac{x}{2\sqrt{Dt}}\right). \tag{8}$$

where

$C(x,t)$ = diffusion species concentration at position x and time t

C_o = concentration of the diffusing species at the free surface (1.0 atoms/m^3)

D = diffusivity (1.0 m^2/s).

The solution of Equation (8) was found using Microsoft Excel™ using the series expansion given in CRC Standard Mathematical Tables and Formulae[5]. This expansion is

$$erfc(x) = 1 - erf(x) = 1 - \frac{2}{\sqrt{\pi}}\left(x - \frac{x^3}{3} + \frac{1}{2!}\frac{x^5}{5} - \frac{1}{3!}\frac{x^7}{7} + \frac{1}{4!}\frac{x^9}{9}\ldots\right). \tag{9}$$

Twenty-five terms were taken in this expansion with the last term contributing less than 1.0×10^{-11} at the full depth of the model.

Two comparisons were made for this model between the values of Equation (8) and results from TMAP7. The first comparison was made for the concentration at times ranging from $t = 0$ to 30 s at a distance from the surface of $x = 0.45$ m. The disagreement between Equation (8) and TMAP7 was less than 0.02% at $t = 1$ sec. The variance decreased with time, declining quickly to 0.001%. These values are listed in Table 2.

The second comparison examined the concentration profile from $x = 0.005$ to 0.195 m at increments of 0.01 m at time, $t = 25$ s. The variance between Equation (8) and TMAP7 is small, exceeding 0.1% only at depths greater than 11 m. The comparison of these values can be seen in Table 3 and in Figure 3.

Table 2. Concentration history at *x* = 0.45 m for problem Val-1b, diffusion in a semi-infinite slab.

Time	TMAP7	Theory	Variation
0	0.00000	0.00000	0.00000
1	0.74926	0.75033	-0.00143
2	0.82158	0.82198	-0.00049
3	0.85402	0.85424	-0.00026
4	0.87345	0.87359	-0.00016
5	0.88674	0.88684	-0.00011
6	0.89656	0.89664	-0.00009
7	0.90421	0.90427	-0.00007
8	0.91038	0.91043	-0.00005
9	0.91549	0.91553	-0.00004
10	0.91981	0.91985	-0.00004
11	0.92354	0.92357	-0.00003
12	0.92678	0.92681	-0.00004
13	0.92965	0.92968	-0.00003
14	0.93221	0.93223	-0.00002
15	0.93450	0.93452	-0.00002
16	0.93658	0.93660	-0.00002
17	0.93847	0.93848	-0.00002
18	0.94020	0.94021	-0.00002
19	0.94179	0.94181	-0.00002
20	0.94326	0.94328	-0.00002
21	0.94463	0.94464	-0.00001
22	0.94590	0.94591	-0.00001
23	0.94709	0.94710	-0.00001
24	0.94820	0.94821	-0.00001
25	0.94925	0.94926	-0.00001
26	0.95023	0.95024	-0.00001
27	0.95116	0.95117	-0.00001
28	0.95204	0.95205	-0.00001
29	0.95287	0.95288	-0.00001
30	0.95367	0.95367	0.00000

Table 3. Concentration Profile (atom/m^3) at *t* = 25 sec for diffusion in a semi-infinite slab.

X (m)	TMAP7	Theory	Variation
0.00	1.00000	1.00000	0.00000
0.05	0.99436	0.99436	0.00000
0.15	0.98307	0.98308	-0.00001
0.25	0.97179	0.97180	-0.00001
0.35	0.96052	0.96052	0.00000
0.45	0.94925	0.94926	-0.00001
0.55	0.93799	0.93800	-0.00001
0.65	0.92675	0.92676	-0.00001
0.75	0.91551	0.91553	-0.00002
0.85	0.90430	0.90432	-0.00002
0.95	0.89311	0.89313	-0.00002
1.05	0.88193	0.88195	-0.00003
1.15	0.87078	0.87081	-0.00003
1.25	0.85966	0.85968	-0.00003
1.35	0.84856	0.84859	-0.00003
1.45	0.83750	0.83752	-0.00003
1.55	0.82646	0.82649	-0.00004
1.65	0.81546	0.81549	-0.00004
1.75	0.80450	0.80453	-0.00004
1.85	0.79357	0.79361	-0.00005
1.95	0.78269	0.78272	-0.00004

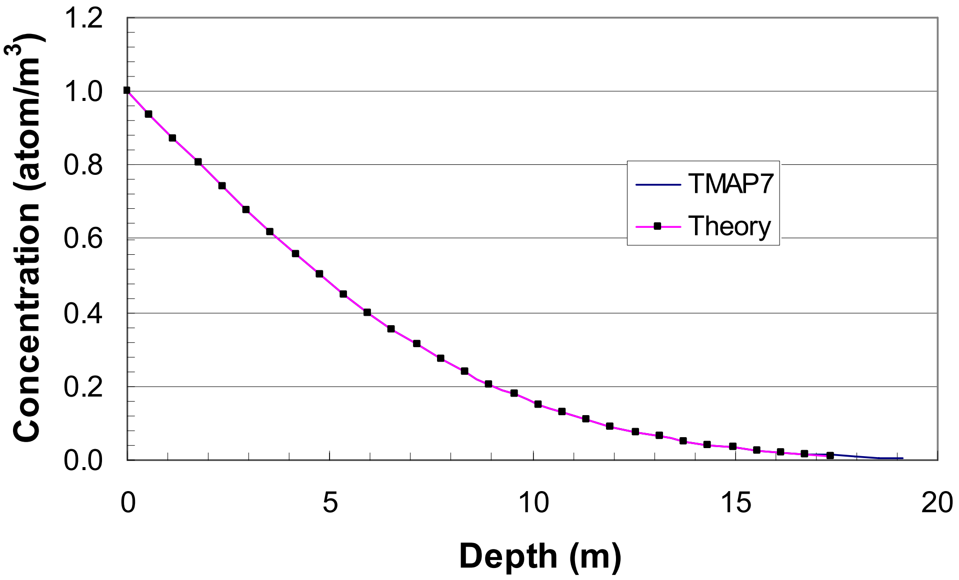

Figure 3. Concentration profile in a semi-infinite slab of SiC after 25 s from problem Val-1b.

The third, and final, comparison for this problem was the comparison of the diffusive flux into the slab. The flux into or out of a slab is proportional to the concentration gradient in the x direction at the slab surface. The solution[6] is given by

$$J = C_o \sqrt{\frac{D}{t\pi}} \exp\left(\frac{x}{2\sqrt{Dt}} \right) \tag{10}$$

The values of Equation (10) were found using Microsoft Excel™. They were compared to the values obtained from TMAP7 and can be seen in Table 4. The variance is never greater than 0.44%.

Table 4. Flux (atom/m^2 sec) into semi-infinite slab from a constant source

Time (s)	TMAP7	Theory	Variance
0	0.00000	0.00000	0.00000
1	0.56668	0.56419	0.00441
2	0.39982	0.39894	0.00220
3	0.32621	0.32574	0.00146
4	0.28240	0.28209	0.00108
5	0.25253	0.25231	0.00086
6	0.23050	0.23033	0.00074
7	0.21338	0.21324	0.00064
8	0.19958	0.19947	0.00055
9	0.18815	0.18806	0.00046
10	0.17849	0.17841	0.00043
11	0.17018	0.17011	0.00041
12	0.16293	0.16287	0.00038
13	0.15653	0.15648	0.00033
14	0.15083	0.15079	0.00029
15	0.14572	0.14567	0.00032
16	0.14109	0.14105	0.00030
17	0.13687	0.13684	0.00025
18	0.13301	0.13298	0.00022
19	0.12946	0.12943	0.00020
20	0.12618	0.12616	0.00019
21	0.12314	0.12312	0.00019
22	0.12031	0.12029	0.00020
23	0.11766	0.11764	0.00016
24	0.11519	0.11516	0.00022
25	0.11286	0.11284	0.00020
26	0.11067	0.11065	0.00021
27	0.10860	0.10858	0.00020
28	0.10664	0.10662	0.00017
29	0.10478	0.10477	0.00012
30	0.10302	0.10301	0.00013

2.3 Problem 1c: Diffusion in a Partially Preloaded Semi-Infinite Slab (Val-1c)

This problem models a semi-infinite slab with the first 10 meters preloaded to a uniform concentration. The concentration at the free surface is set to zero for time, $t \geq 0$ sec, when the pre-loaded inventory is allowed to diffuse out the surface and through the slab. No traps are assumed to be present. Comparisons are made between TMAP7 and analytical values for concentration histories at two locations: one in the initially unloaded region of the slab, at $x = 12$ m, and one near the surface, $x = 0.25$ m. A third is made at the end of the preloaded region.

By analogy with Carslaw and Jaeger[7] the concentration as a function of space and time is

$$C = \frac{C_o}{2}\left[2erf\left(\frac{x}{2\sqrt{Dt}}\right) - erf\left(\frac{x-h}{2\sqrt{Dt}}\right) - erf\left(\frac{h+x}{2\sqrt{Dt}}\right)\right] \tag{11}$$

where

h = thickness of pre-loaded region in the slab (10 m)

C_o = concentration of pre-loaded section (1.0 atoms/m^3)

D = diffusion coefficient (1.0 m^2/sec)

Results for the concentration history at $x = 12$ m can be seen in Table 5. Even for very short times when the theoretical solution has difficulty with evaluation, the variance for this problem never exceededs 0.3%.

Time (s)	Tmap7	Theory	Variance
0	0.00000	0	1
5	0.26268	0.26340	-0.002722
10	0.31901	0.32007	-0.003313
15	0.32806	0.32907	-0.003070
20	0.31762	0.31839	-0.002426
25	0.29938	0.29989	-0.001731
30	0.27872	0.27905	-0.001185
35	0.25813	0.25832	-0.000742
40	0.23868	0.23877	-0.000387
45	0.22078	0.22081	-0.000130
50	0.20452	0.20450	0.000076
55	0.18984	0.18979	0.000219
60	0.17661	0.17655	0.000344
65	0.16470	0.16463	0.000445
70	0.15397	0.15388	0.000544
75	0.14426	0.14418	0.000565
80	0.13548	0.13540	0.000613
85	0.12752	0.12743	0.000674
90	0.12026	0.12018	0.000662
95	0.11365	0.11357	0.000672
100	0.10760	0.10752	0.000678

Table 5. Concentration history at $x = 12$ meters.

The next comparison for this model is at *x* = 0.5 m, the closest node to the surface. The variance for this problem was less than 1 % for times, $t \geq 15$ sec. Again, at short times the theoretical solution is imprecise. These values can be seen in Table 6.

Time (s)	Tmap7	Theory	Variance
0	0.00000	0	1
5	0.12689	0.12475	0.017147
10	0.08250	0.08164	0.010581
15	0.05951	0.05893	0.009809
20	0.04532	0.04491	0.009146
25	0.03590	0.03560	0.008446
30	0.02930	0.02907	0.007776
35	0.02448	0.02431	0.007129
40	0.02084	0.02070	0.006595
45	0.01801	0.01790	0.006093
50	0.01577	0.01568	0.005705
55	0.01395	0.01388	0.005317
60	0.01246	0.01240	0.004951
65	0.01122	0.01116	0.004723
70	0.01016	0.01012	0.004443
75	0.00927	0.00923	0.004196
80	0.00849	0.00846	0.003989
85	0.00782	0.00779	0.003788
90	0.00723	0.00721	0.003620
95	0.00672	0.00669	0.003463
100	0.00626	0.00624	0.003315

Table 6. Concentration at *x* = 0.5 meters

The last comparison is made at *x* = h. For this case, Equation (11) reduces to

$$C = \frac{C_o}{2}\left[2erf\left(\frac{h}{2\sqrt{Dt}}\right) - erf\left(\frac{h+x}{2\sqrt{Dt}}\right)\right]. \qquad (12)$$

The variance between the values obtained from TMAP7 and Equation (12) has the largest values at times, $t \leq 20$ sec. For all other times, the variance is less than 0.1 %. The comparison of TMAP7 calculated values with theory may be seen in Table 7.

Time (s)	Tmap7	Theory	Variance
0	0.00000	0	1
5	0.49780	0.49843	-0.001283
10	0.47344	0.47466	-0.002574
15	0.43138	0.43224	-0.002004
20	0.38646	0.38694	-0.001244
25	0.34482	0.34504	-0.000637
30	0.30816	0.30821	-0.000166
35	0.27647	0.27642	0.000177
40	0.24923	0.24912	0.000417
45	0.22580	0.22567	0.000590
50	0.20559	0.20544	0.000732

Table 7. Concentration at *x* = 10 meters

2.4 Problem 1d: Permeation Problem with Trapping (Val-1da, Val-1db, Val-1dc)

The following three models simulate diffusion through a slab in which traps are operational. The three trapping regimes demonstrated are an effective diffusivity trap, a strong trap, and a set of three traps in the effective diffusivity range with different trap strengths. The diffusion boundary conditions for this set of problems are fixed-concentration or *sconc*, with one surface kept at a constant non-zero concentration and the other set at zero concentration. Initially, the slab is empty. Validation criteria for these problems will be the comparison of the flux and breakthrough times for each of the models with idealizations. The breakthrough time of the flux may have one of two limiting values, which depend on whether the trapping is in the effective diffusivity or strong-trapping regime. A trapping parameter (see Appendix B) is defined by

$$\zeta = \frac{\lambda^2 \upsilon}{D_o \rho} \exp\left(\frac{E_d - \varepsilon}{kT}\right) + \frac{c}{\rho} \tag{13}$$

where

λ = lattice parameter (assume 3.162 x 10^{-8} m)

ν = Debye frequency (1 x 10^{13} s^{-1})

ρ = trapping site fraction (0.1)

D_o = diffusivity pre-exponential (1 m^2/sec)

E_d = diffusion activation energy (assume 0 eV)

ε = trap energy

k = Boltzmann's constant

T = temperature (1000 K)

c = mobile atom concentration

The determining value for which regime is dominant is the relation of ζ to c/ρ (0.0001 here).

2.4.1 Effective Diffusivity Trap (Val-1da, Val-1dd)

If $\zeta >> c/\rho$, then the effective diffusivity regime applies, and the flux transient is nearly identical to the standard diffusion transient, but with the diffusivity replaced by an effective diffusivity,

$$D_{eff} = \frac{D}{1+\sum_{i} \frac{1}{\varsigma_i}} \tag{14}$$

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

$$\tau_{b_e} = \frac{l^2}{2\pi^2 D_{eff}} \tag{15}$$

where

l = thickness of slab (1 m)

D_{eff} = effective diffusivity of gas (m^2/s).

The permeation transient is then given by

$$J_p = \frac{c_o D}{l}\left[1+2\sum_{m=1}^{\infty}(-1)^m \exp\left(-m^2 \frac{t}{\tau_{b_e}}\right)\right] \tag{16}$$

where τ_{be} is as defined in Equation (15).

The first example is the case where a single trap is in the effective diffusivity limit. The ratio ε/k (see Equation (13)) was taken as 100, to give a value of $\zeta = 90.49\ c/\rho$. TMAP7's breakthrough time was found numerically by using a three-point differentiation method given by Fogler[8] to find the steepest slope.

$$\left(\frac{dC_A}{dt}\right)_{t_i} = \frac{1}{2\Delta t}\left[C_{A(i+1)} - C_{A(i-1)}\right] \approx m \tag{17}$$

Then, the point where the slope was the steepest was used with the slope at that point to find the intersection with the time axis. This was computed to be 0.604 seconds. The analytical breakthrough time (plotted) was calculated to be 0.607 seconds. The variance between theoretical values of the permeation flux and those calculated by TMAP7 using this model is less than 1%, for times greater than 1 second, as shown in Figure 4. The permeation curve where no trapping is present (Val-1dd) is also shown in Figure 4 to illustrate the retarding of the permeation curve by a trap.

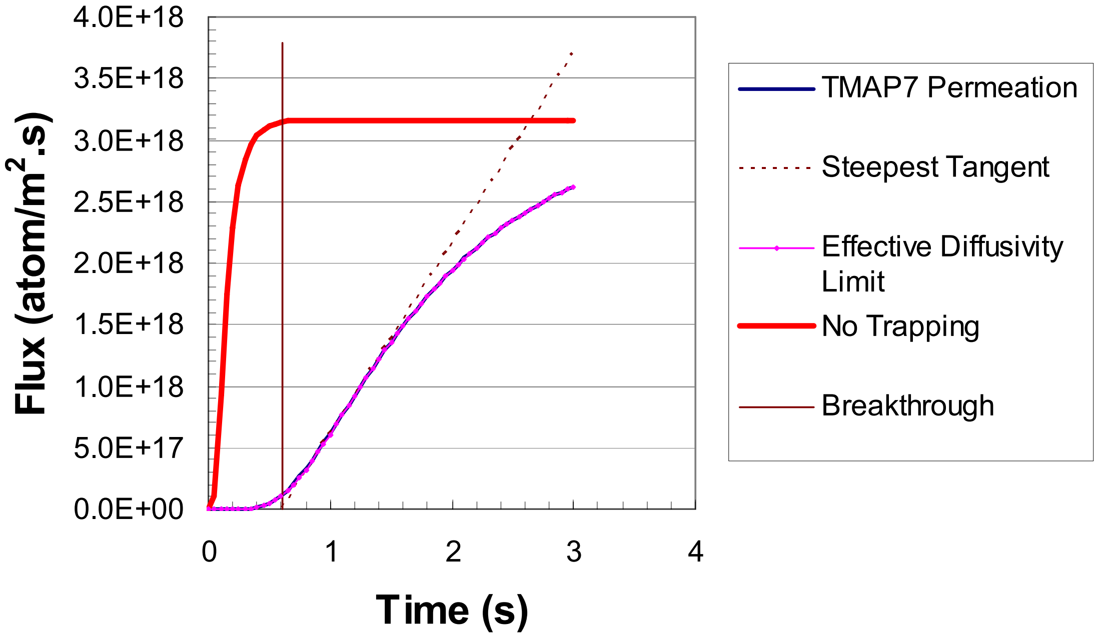

Figure 4. Effective-diffusivity, single trap (Val-1da).

2.4.2 Strong Trap (Val-1db)

In the second model, $\zeta \approx c/\rho$, is applied to obtain a strong trapping regime. In this regime, no permeation occurs until essentially all the traps have been filled. Then the permeation rapidly turns on to its steady state value. The breakthrough time is given by

$$\tau_{b_d} = \frac{l^2 \rho}{2 c_o D} \tag{18}$$

where c_o, ρ, l, and D are defined as in the first model. The value of ε/k is taken to be 100,000 K, to give $\zeta \frac{\rho}{c} - 1 = 3.72 \times 10^{-41}$. The only difference in the input file between the first and second models is this parameter and a larger time step.

The permeation curve for TMAP7 calculation using this model can be seen in Figure 5. The breakthrough time in the strong trapping regime was taken as the first time that the permeation was at 99% of its steady state value. This occurred at 500 seconds. The estimated breakthrough time from Equation (18) is 500 seconds (vertical line in Figure 5). Note that the rise is really more abrupt than shown in Figure 5. The relative slope is due to the finite data spacing in the plotting lists.

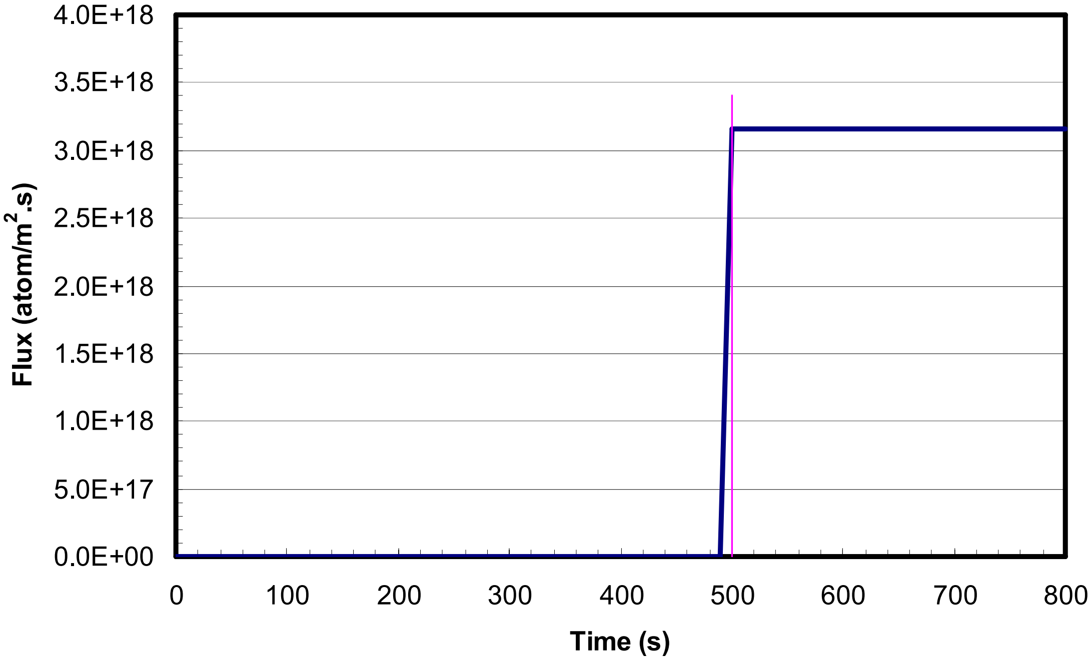

Figure 5. Permeation for strong-trapping regime (Val-1db)

2.4.3 Multiple Trap (Val-1dc)

The last problem modeled in this section demonstrates the effects of multiple traps. This feature illustrates TMAP7's capabilities to allow for multiple traps. Three traps that are relatively weak are assumed to be active in a slab. The parameters of the first trap are the same as the trap in the effective diffusivity limit, first model. The second and third traps vary by having trap concentrations of 0.15 and 0.20 atom fractions and the values of ε/k chosen to be 500 K and 800 K, respectively. These values give the following values for ζ:

Trap 1: 0.09048 c/ρ

Trap 2: 0.04044 c/ρ

Trap 3: 0.02247 c/ρ.

The effective diffusivity was calculated from Equation (14), D_{eff} = 0.01242 m^2/sec, and the breakthrough time was calculated from Equation (15) to be 4.12 sec. TMAP7's calculated breakthrough time was 3.93 sec. The permeation curves that were calculated using Equation (16) are compared with TMAP7 results in Figure 6. The graphs for the theoretical flux and the calculated flux are in good agreement.

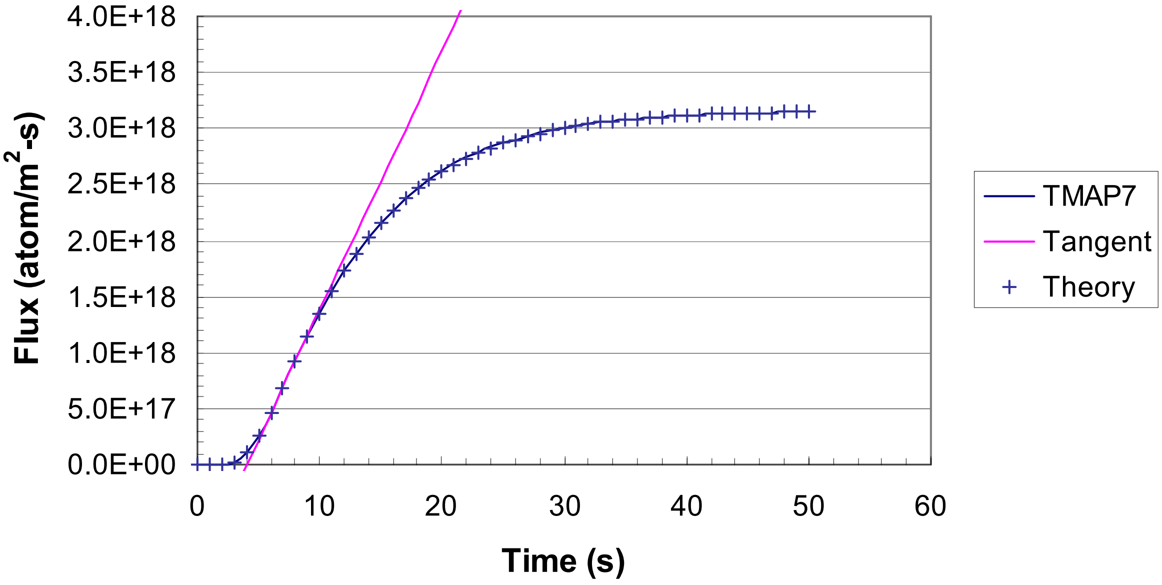

Figure 6. Permeation curve for slab with multiple traps (Val-1dc).

2.5 Problem 1e: Diffusion with Composite Material Layers (Val-1e)

A composite structure of PyC and SiC is modeled with a constant concentration boundary condition on the free surface of the PyC and a zero-concentration boundary on the free surface of the SiC. The concentration profile in steady state is to be analyzed. The steady-state solution for the PyC is given in Equation (19)

$$C = C_o\left[1+\frac{x}{l}\left(\frac{D_{PyC}a}{aD_{PyC}+lD_{SiC}}-1\right)\right] \tag{19}$$

while the concentration profile for the SiC is given by

$$C = C_o\left(\frac{a+l-x}{l}\right)\left(\frac{D_{PyC}a}{aD_{PyC}+lD_{SiC}}\right) \tag{20}$$

where

a = thickness of the PyC layer (33 μm)

l = thickness of the SiC layer (66 μm)

C_o = the concentration at the surface (3.0537 x 10^{25} atoms/m^3)

S_a = Solubility of both species was taken as 1.0 (units arbitrary)

The values for the diffusivity were taken as constants, D_{PyC} = 1.274 x 10^{-7} $m^{2/}$sec and D_{SiC}=2.622 x 10^{-11} m^2/sec. The variance for this problem does not exceed 0.6%. The comparison of Equations (19) and (20) with TMAP7's values can be seen in Table 8.

Table 8. Steady-state concentration profile in composite slab

x (m)	TMAP7	Theory	Variance
0.000E+00	3.0537E+25	3.0537E+25	0.00000
1.500E-06	3.0537E+25	3.0537E+25	-0.00001
5.500E-06	3.0536E+25	3.0536E+25	0.00000
1.050E-05	3.0536E+25	3.0535E+25	-0.00003
1.550E-05	3.0536E+25	3.0534E+25	-0.00006
2.050E-05	3.0535E+25	3.0533E+25	-0.00006
2.550E-05	3.0535E+25	3.0532E+25	-0.00009
3.050E-05	3.0534E+25	3.0531E+25	-0.00009
3.300E-05	3.0534E+25	3.0531E+25	-0.00011
3.300E-05	3.0534E+25	3.0524E+25	-0.00031
3.825E-05	2.8090E+25	2.8096E+25	0.00023
4.875E-05	2.3205E+25	2.3240E+25	0.00151
5.925E-05	1.8330E+25	1.8384E+25	0.00294
6.975E-05	1.3471E+25	1.3528E+25	0.00420
8.025E-05	8.6257E+24	8.6717E+24	0.00531
9.075E-05	3.7927E+24	3.8156E+24	0.00599
9.750E-05	6.8954E+23	6.9374E+23	0.00605
9.900E-05	0.0000E+00	0.0000E+00	0.00000

Demonstration of transient agreement with theory may also be shown by examining the concentration history at an arbitrary point (we choose 15.75 μm into the SiC layer) as a function of time given that, initially, both PyC and SiC were empty of gas. The transient solution for concentration in the SiC side of the composite slab is

$$C = C_o \left\{ \frac{D_{PyC}(l-x)}{lD_{PyC} + aD_{SiC}} - 2\sum_{n=1}^{\infty} \frac{\sin(a\lambda_n)\sin(kl\lambda_n)\sin[k(l-x)\lambda_n]}{\lambda_n\left[a\sin^2(kl\lambda_n) + l\sin^2(a\lambda_n)\right]} \exp\left(-D_{PyC}\lambda_n^2 t\right) \right\} \tag{21}$$

where

a = thickness of PyC (33 μm)

l = Thickness of SiC (63 μm)

$$k = \sqrt{\frac{D_{PyC}}{D_{SiC}}} = 69.7036$$

and the λ_n are the roots of

$$\tan(\lambda\, a) + k\tan(k\,\lambda\, l) = 0 \tag{22}$$

Figure 7 shows the graphical comparison, and Table 9 lists discreet values and variance. The fit would be better with a finer spatial mesh.

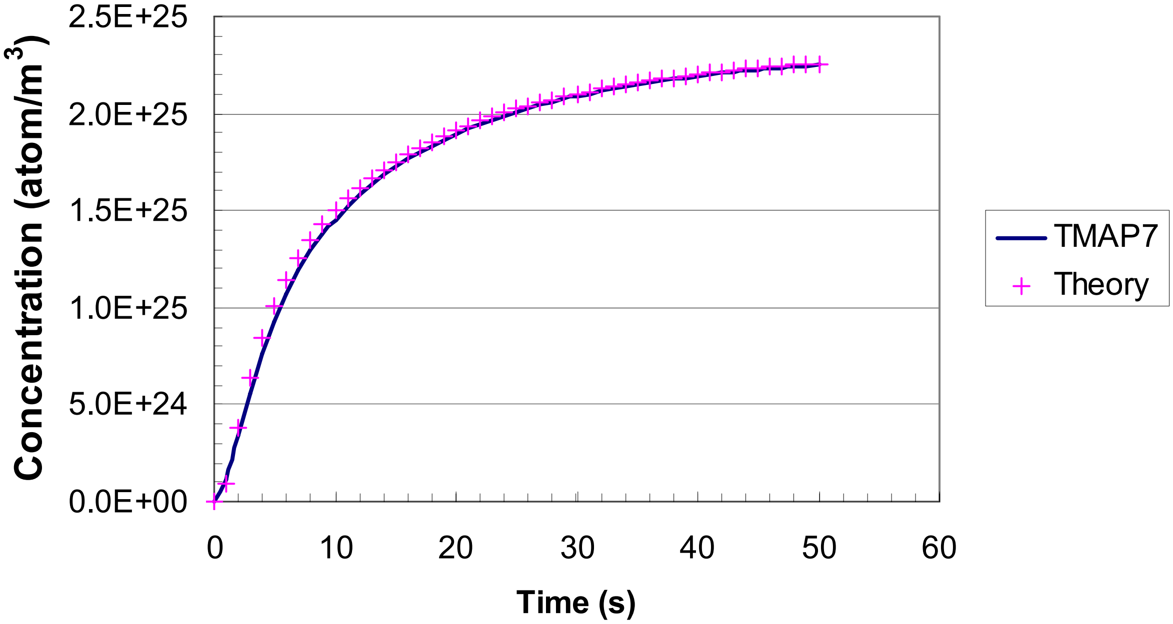

Figure 7. Concentration history 15.75 µm into the SiC layer of a PyC/SiC composite structure (Val-1e).

Table 9. Variance for transient solution in composite slab.

Time	TMAP7	Theory	Variance
0	0.00E+00	0	0
1	1.18E+24	8.92E+23	-0.31841
2	3.37E+24	3.77E+24	0.10697
3	5.60E+24	6.37E+24	0.12112
4	7.59E+24	8.44E+24	0.10116
5	9.27E+24	1.01E+25	0.08061
6	1.07E+25	1.14E+25	0.06416
7	1.19E+25	1.25E+25	0.05172
8	1.29E+25	1.35E+25	0.04242
9	1.38E+25	1.43E+25	0.03535
10	1.46E+25	1.50E+25	0.02987
11	1.52E+25	1.56E+25	0.02566
12	1.58E+25	1.62E+25	0.02230
13	1.64E+25	1.67E+25	0.01959
14	1.68E+25	1.71E+25	0.01736
15	1.73E+25	1.75E+25	0.01551
16	1.77E+25	1.79E+25	0.01399
17	1.80E+25	1.82E+25	0.01272
18	1.83E+25	1.86E+25	0.01164
19	1.87E+25	1.89E+25	0.01072
20	1.89E+25	1.91E+25	0.00993
21	1.92E+25	1.94E+25	0.00922
22	1.94E+25	1.96E+25	0.00863
23	1.97E+25	1.98E+25	0.00808

Time	TMAP7	Theory	Variance
24	1.99E+25	2.00E+25	0.00758
25	2.01E+25	2.02E+25	0.00714
26	2.03E+25	2.04E+25	0.00676
27	2.04E+25	2.06E+25	0.00644
28	2.06E+25	2.07E+25	0.00610
29	2.07E+25	2.09E+25	0.00580
30	2.09E+25	2.10E+25	0.00555
31	2.10E+25	2.11E+25	0.00530
32	2.12E+25	2.13E+25	0.00505
33	2.13E+25	2.14E+25	0.00481
34	2.14E+25	2.15E+25	0.00462
35	2.15E+25	2.16E+25	0.00441
36	2.16E+25	2.17E+25	0.00421
37	2.17E+25	2.18E+25	0.00403
38	2.18E+25	2.19E+25	0.00389
39	2.19E+25	2.19E+25	0.00370
40	2.19E+25	2.20E+25	0.00358
41	2.20E+25	2.21E+25	0.00340
42	2.21E+25	2.22E+25	0.00325
43	2.21E+25	2.22E+25	0.00316
44	2.22E+25	2.23E+25	0.00300
45	2.23E+25	2.23E+25	0.00290
46	2.23E+25	2.24E+25	0.00276
47	2.24E+25	2.24E+25	0.00265
48	2.24E+25	2.25E+25	0.00255
49	2.25E+25	2.25E+25	0.00242
50	2.25E+25	2.26E+25	0.00231

2.6 Problem 1f: Heat Sink/Source Problem

Heat transfer models were set up to validate the heat transfer capabilities of the TMAP7 code. The four problems solved include (a) heat conduction with generation; (b) transient conduction and steady state values in a composite structure, and (c) heating of a semi-infinite slab by convection, and (d) convective heating.

2.6.1 Heat conduction with generation (Val-1fa, Val-1fap)

To model the first problem, the thermal boundary conditions were set so one surface was adiabatic, while the other was kept at constant temperature. The heat generation in the slab was assumed to be constant throughout. Incropera and DeWitt[9] give the analytical solution for the steady state temperature of this model as

$$T = T_s + \frac{QL^2}{2k}\left(1 - \frac{x^2}{L^2}\right) \qquad (23)$$

where

Q = internal heat generation rate (10,000 W/m^3)

L = thickness of slab (1.6 m)

k = thermal conductivity (10 W/m K)

T_s = surface temperature (300 K)

A value for thermal mass, the product of material mass density and specific heat, must be added for TMAP7 thermal calculations. In this problem, $\rho c_p = 1$ J/m^{3}K was assumed. Initially, 16 spatial segments were assumed. The variance for this problem was less than 0.2% for distances less than 1.35 m, but it increased as the distance from the adiabatic surface was increased. To show that this can be reduced with a decrease in the distance between nodes, an additional calculation was performed with 48 spatial segments. The variance was reduced by a factor of approximately 10. The comparison of Equation (23) with TMAP7 values can be seen in Table 10.

Table 10. Heat Conduction with Generation

Position	Theory	16 Segs	Variance	48 Segs	Variance
0	1580	1580	1.439E-16	1580	1.439E-16
0.05	1579	1580	-0.000792	1579	-0.000095
0.15	1569	1570	-0.000797	1569	-0.000096
0.25	1549	1550	-0.000807	1549	-0.000097
0.35	1519	1520	-0.000823	1519	-0.000099
0.45	1479	1480	-0.000845	1479	-0.000101
0.55	1429	1430	-0.000875	1429	-0.000105
0.65	1369	1370	-0.000913	1369	-0.000110
0.75	1299	1300	-0.000962	1299	-0.000115
0.85	1219	1220	-0.001026	1219	-0.000123
0.95	1129	1130	-0.001107	1129	-0.000133
1.05	1029	1030	-0.001215	1029	-0.000146
1.15	919	920	-0.001361	919	-0.000141
1.25	799	800	-0.001565	799	-0.000163
1.35	669	670	-0.001869	669	-0.000194
1.45	529	530	-0.002364	529	-0.000246
1.55	379	380	-0.003300	379	-0.000370
1.60	300	300	0.000000	300	0.000000

2.6.2 Thermal Diffusion Transient (Val-1fb)

The second problem validates the thermal diffusion capability in a slab. The temperature of the left side of the thermal segment was held constant at 400 K while the right side was held at a constant 300 K. The initial temperature in the slab was 300 K. For this example, the thickness, L, was 3.75 m and the heat production rate was $Q = 0$. Diffusion was ignored by setting the mobile species concentration to zero and using non-flow boundaries. The analytical solution is given by

$$T(x,t) = T_o + (T_1 - T_o)\left[1 - \frac{x}{L} - \frac{2}{L}\sum_{m=0}^{\infty}\frac{1}{\lambda_m}\sin(\lambda_m x)\exp\left(-\alpha\lambda_m^2 t\right)\right] \tag{24}$$

where

$$\lambda_m = m\frac{\pi}{L} \tag{25}$$

and thermal diffusivity is

$$\alpha = \frac{k}{C_p \rho} \tag{26}$$

For the problem analyzed,

$\alpha = 1.0\ m^2/s$,

$T_o = 300$ K, and

$T_1 = 400$ K.

The values for Equation (24) were found using Microsoft Excel™. The last term in the summation taken contributed less than 1 x 10^{-13} of the theoretical value. The agreement between TMAP7 and Equation (24) is excellent, with the variance less than 0.01 % for each case tested. The comparison between the values can be seen in Figure 8 for temperature profiles through the slab at 0.1, 0.5, 1.0, and 5.0 seconds.

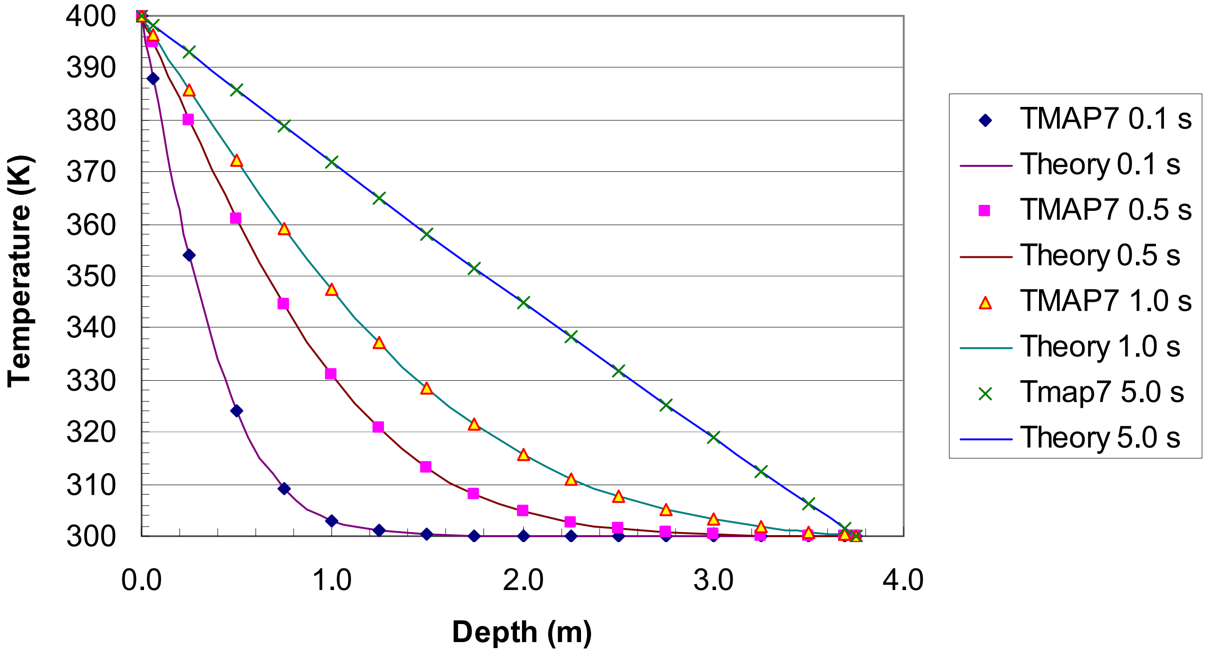

Figure 8. Transient temperature distribution for various times in a slab (Val-1fb).

2.6.3 Problem 1fc: Conduction in composite structure with constant surface temperatures (Val-1fc, Val-1fcs)

The third heat transfer problem studied was heat transfer through a composite with constant surface temperatures. The composite was a 40-cm thick layer of Cu followed by a 40-cm layer of Fe. The temperature of both layers was initially 0 K, but at time *t* = 0, the outside face of the copper was held at 600 K while the outside face of the Fe was maintained at 0 K. This problem by TMAP7 for both the transient and steady state solutions were compared to values obtained from ABAQUS.[10] The ABAQUS code was setup and run by R. G. Ambrosek. ABAQUS is a heat transfer program that has been validated for both transient and steady state solutions. The transient solution was compared at a constant time and at constant distance. The constant time comparison between ABAQUS and TMAP7 was made at time, t = 150 sec. The variance in this comparison grows with increasing distance. This may be due to the time interval on both programs being larger than needed, or round-off error from the printed values. The constant time values can be seen in Table 11.

Table 11. Temperature distribution in composite structure at t = 150 seconds (Val-1fc).

Distance (m)	ABAQUS	TMAP7	Variance
0	600.00	600.000	0.00000
0.01	574.37	574.400	-0.00005
0.03	523.40	523.600	-0.00038
0.05	473.30	473.600	-0.00063
0.07	424.63	425.100	-0.00111
0.09	377.88	378.400	-0.00137
0.11	333.50	334.100	-0.00180
0.13	291.85	292.500	-0.00222
0.15	253.20	253.900	-0.00276
0.17	217.77	218.500	-0.00334
0.19	185.67	186.400	-0.00392
0.21	156.93	157.700	-0.00488
0.23	131.51	132.200	-0.00522
0.25	109.32	110.000	-0.00618
0.27	90.20	90.790	-0.00651
0.29	73.98	74.480	-0.00678
0.31	60.44	60.860	-0.00692
0.33	49.37	49.690	-0.00636
0.35	40.56	40.770	-0.00505

The constant distance values were compared at x = 0.09 m, at 5 second intervals from time t = 0 to 150 sec. These results can be seen in Table 12. The variance is initially large, but reduces as the time increases. The initially large variance may be due to the same factors of spatial resolution and time step size mentioned earlier.

Table 12. Temperature distribution in composite structure at x = 0.09 meters (Val-1fc)

Time (s)	TMAP 7	ABAQUS	Variance
0	0.00	0	0.0000
5	6.50	10.11	-0.3569
10	37.03	43.47	-0.1482
15	75.11	81.42	-0.0775
20	110.42	115.90	-0.0473
25	140.99	145.60	-0.0317
30	167.17	171.10	-0.0230
35	189.68	193.10	-0.0177
40	209.20	212.10	-0.0137
45	226.29	228.90	-0.0114
50	241.39	243.70	-0.0095
55	254.84	256.90	-0.0080
60	266.91	268.70	-0.0067
65	277.82	279.50	-0.0060
70	287.74	289.36	-0.0056
75	296.81	298.30	-0.0050
80	305.14	306.40	-0.0041
85	312.83	314.00	-0.0037
90	319.95	321.00	-0.0033
95	326.57	327.60	-0.0031
100	332.74	333.70	-0.0029
105	338.52	339.40	-0.0026
110	343.94	344.80	-0.0025
115	349.04	349.80	-0.0022
120	353.85	354.60	-0.0021
125	358.39	359.10	-0.0020
130	362.70	363.40	-0.0019
135	366.78	367.40	-0.0017
140	370.66	371.30	-0.0017
145	374.36	374.90	-0.0014
150	377.89	378.40	-0.0013

The steady-state solution for this problem was compared to the analytical solution in addition to the ABAQUS answer. To solve for the steady state solution for this problem, the heat flux is given by

$$q'' = \frac{T_{S_A} - T_{S_B}}{\frac{L_A}{k_A} + \frac{L_B}{k_B}} \tag{27}$$

where

T_{si} = Temperature of surface i, left (A) and right (B),

L_i = Length of segment i

k_i = thermal conductivity of segment i.

For the solution to be at steady state, the flux in and out of any section of the slab must be equal. The temperature at the interface can be found by setting the flux through *A* equal to the flux through *B*.

$$\frac{T_{S_A} - T_I}{\frac{L_A}{k_A}} = \frac{T_I - T_{S_B}}{\frac{L_B}{k_B}} \tag{28}$$

where

T_I = temperature of interface,

k_A = 401 W /m K,

k_B = 80.2 W /m K,

$L_A = L_B$ = 0.4 meters,

T_{S_A} = 600 K

T_{S_B} = 0 K

From Equation (28), the interface temperature is found to be T_I = 500 K. The temperature profile for conduction in steady state, with constant physical properties, is linear. The temperature profile of A and B can be found through linear interpolation. The comparison of TMAP7, ABAQUS, and the analytical solution were found to be identical. These values can be seen in Table 13.

Table 13. Steady-state temperature distribution for composite structure

Distance (m)	Tmap7	ABAQUS	Variance
0	600.00	600.000	0.00000
0.01	574.37	574.400	-0.00005
0.03	523.40	523.600	-0.00038
0.05	473.30	473.600	-0.00063
0.07	424.63	425.100	-0.00111
0.09	377.88	378.400	-0.00137
0.11	333.50	334.100	-0.00180
0.13	291.85	292.500	-0.00222
0.15	253.20	253.900	-0.00276
0.17	217.77	218.500	-0.00334
0.19	185.67	186.400	-0.00392
0.21	156.93	157.700	-0.00488
0.23	131.51	132.200	-0.00522
0.25	109.32	110.000	-0.00618
0.27	90.20	90.790	-0.00651
0.29	73.98	74.480	-0.00678
0.31	60.44	60.860	-0.00692
0.33	49.37	49.690	-0.00636
0.35	40.56	40.770	-0.00505

2.6.4 Problem 1fd: Convective Heating (Val-1fd)

The fourth heat transfer problem modeled was the heating of a semi-infinite slab by convection at the boundary. The slab was initially configured with a constant temperature of 100 K throughout the slab. A convection boundary was then activated at the surface for time, t ≥ 0 sec. Incorpera and DeWitt[9] give for the solution

$$T(x,t) = T_i + (T_\infty - T_i)\left\{\left[erfc\left(\frac{x}{2\sqrt{t\alpha}}\right)\right] - \left[\exp\left(\frac{hx}{k} + \frac{h^2 t\alpha}{k^2}\right)\right]\left[erfc\left(\frac{x}{2\sqrt{t\alpha}} + \frac{h\sqrt{t\alpha}}{k}\right)\right]\right\} \quad (29)$$

where

T_i = initial temperature (100 K)

T_∞ = temperature of enclosure (500 K)

h = conduction coefficient (200 W/m^2 K)

k = thermal conductivity (801 W/m K)

α = thermal diffusivity (1.17 x 10^{-4} m^2/s)

The depth x of 5 cm was used for comparison. Values of the complimentary error function were computed using a series expansion in Microsoft Excel™. The last term computed contributed less than 1.0 x 10^{-120}. The variance between Equation (29) and TMAP7 was less than 0.2%, for all times greater than 30 sec, as can be seen in Table 14. A graphical comparison can be seen in Figure 9.

Table 14. Heating of Semi-Infinite Slab by Convection

Time (s)	TMAP 7	Theory	Variance
0	100.00	100.0000	0.00000
10	102.14	100.0000	0.02140
20	104.06	103.6389	0.00406
30	105.80	105.5492	0.00238
40	107.39	107.2521	0.00129
50	108.86	108.7947	0.00060
60	110.23	110.2114	0.00017
70	111.51	111.5265	-0.00015
80	112.72	112.7576	-0.00033
90	113.86	113.9178	-0.00051
100	114.94	115.0174	-0.00067
110	115.98	116.0641	-0.00072
120	116.97	117.0644	-0.00081
130	117.92	118.0234	-0.00088
140	118.84	118.9455	-0.00089
150	119.72	119.8342	-0.00095
160	120.58	120.6927	-0.00093
170	121.41	121.5235	-0.00093
180	122.21	122.3290	-0.00097

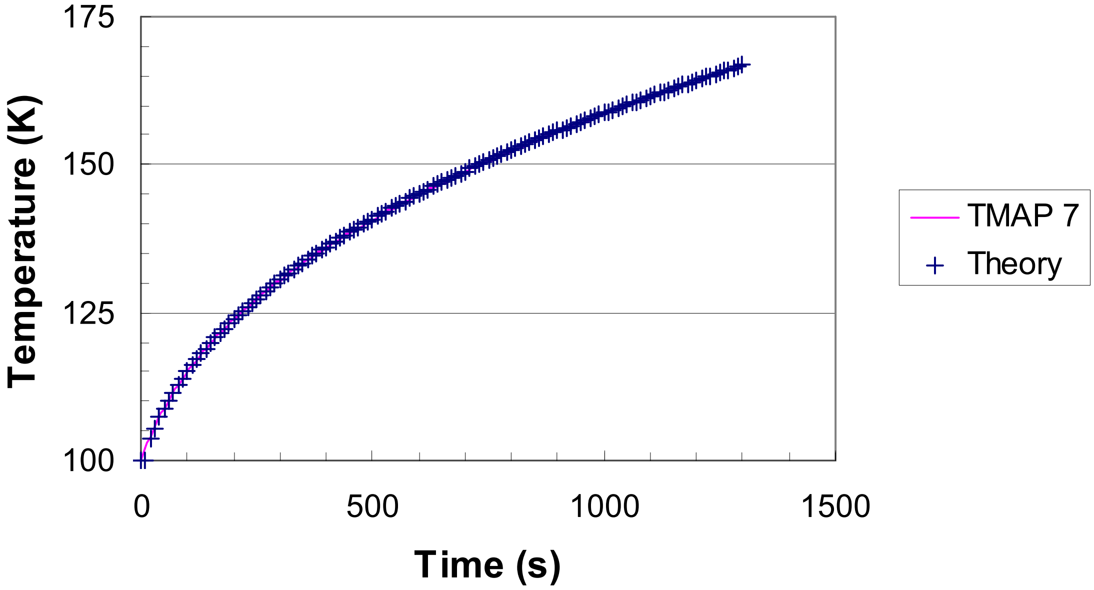

Figure 9. Convective heating at depth 5 cm in a semi-infinite slab (Val-1fd)

2.7 Problem 1g: Enclosure Reaction Problems

Three problems were solved in TMAP7 to test its capability to handle enclosure reactions. The first model is a simple forward reaction with two reactants forming one product. In the first model, the reactants start in their stoichiometric ratio. The second problem varies from the first in that the concentrations of the reactants vary from their stoichiometric ratio. The third problem examines a series reaction.

2.7.1 Simple Forward Reactions (Val-1ga and Val-1gb)

The first and second problems consider the simple chemical reaction

$$A + B \rightarrow AB . \tag{30}$$

The rate at which the concentrations change (rate of reaction) is assumed first order with respect to the concentrations of A and B. The rate coefficient, K_r, is a constant for the reaction and has no spatial or time dependence. The simple forward reaction rate

$$\frac{dC_{AB}}{dt} = R_c = K_r C_A C_B \tag{31}$$

is positive if AB is produced and negative if AB is consumed in the reaction. This may also be written

$$\frac{dC_{AB}}{\left(C_{AB} - C_{A_0}\right)\left(C_{AB} - C_{B_0}\right)} = K_r dt \tag{32}$$

The solution for this problem is[11]

$$C_{AB} = C_{A_o} \left\{ \frac{1-\exp\left[K_R t\left(C_{A_O} - C_{B_O}\right)\right]}{1-\dfrac{C_{A_O}}{C_{B_O}}\exp\left[K_R t\left(C_{A_O} - C_{B_O}\right)\right]} \right\} \tag{33}$$

where

C_{AB} = concentration of species [AB]

C_{A_O} = initial concentration of species [A], assumed greater than C_{B_O} C_{B_O} = initial concentration of species [B]

If $C_{A_o} = C_{B_O}$, Equation (32) is solved by

$$C_{AB} = C_{A_O} - \frac{1}{\dfrac{1}{C_{A_O}} + K_R t} . \tag{34}$$

The analytical solutions of Equations (33) and (34) were found and compared to the values obtained from TMAP7. Equation (34) was solved and compared to TMAP7 for problem Val-1ga, where the starting pressures of species [A] and [B] were equal at 1.0E-06 Pa. Equation (33) was compared to TMAP7 for problem Val-1gb where the starting pressures of the reacting species were 1.0E-6 Pa for [A] and 5.0e-7 Pa for [B]. In each case, K_r was 4.14E-15 m^3/s. These results are listed in Table 15. Figure 10 shows a graphical comparison of the two cases. The variance in each of the two cases drops below 0.2% for time, $t \geq 2$ sec.

Table 15. Concentration of product for equal and unequal starting concentrations.

Equal Starting Pressures			**Unequal Starting Pressures**		
TMAP7	**Theory**	**Variance**	**TMAP7**	**Theory**	**Variance**
0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1.2030E+14	1.2077E+14	-0.00392	1.4932E+13	1.4942E+13	-0.00063
1.6067E+14	1.6103E+14	-0.00222	2.0493E+13	2.0501E+13	-0.00038
1.8088E+14	1.8116E+14	-0.00153	2.2678E+13	2.2684E+13	-0.00026
1.9301E+14	1.9324E+14	-0.00117	2.3554E+13	2.3559E+13	-0.00021
2.0110E+14	2.0129E+14	-0.00095	2.3909E+13	2.3913E+13	-0.00017
2.0687E+14	2.0704E+14	-0.00081	2.4053E+13	2.4056E+13	-0.00015
2.1120E+14	2.1135E+14	-0.00072	2.4111E+13	2.4115E+13	-0.00015
2.1457E+14	2.1471E+14	-0.00064	2.4135E+13	2.4138E+13	-0.00015
2.1726E+14	2.1739E+14	-0.00059	2.4144E+13	2.4148E+13	-0.00015
2.1947E+14	2.1959E+14	-0.00054	2.4148E+13	2.4152E+13	-0.00015
2.2130E+14	2.2142E+14	-0.00051	2.4150E+13	2.4153E+13	-0.00014
2.2286E+14	2.2297E+14	-0.00048	2.4151E+13	2.4154E+13	-0.00014

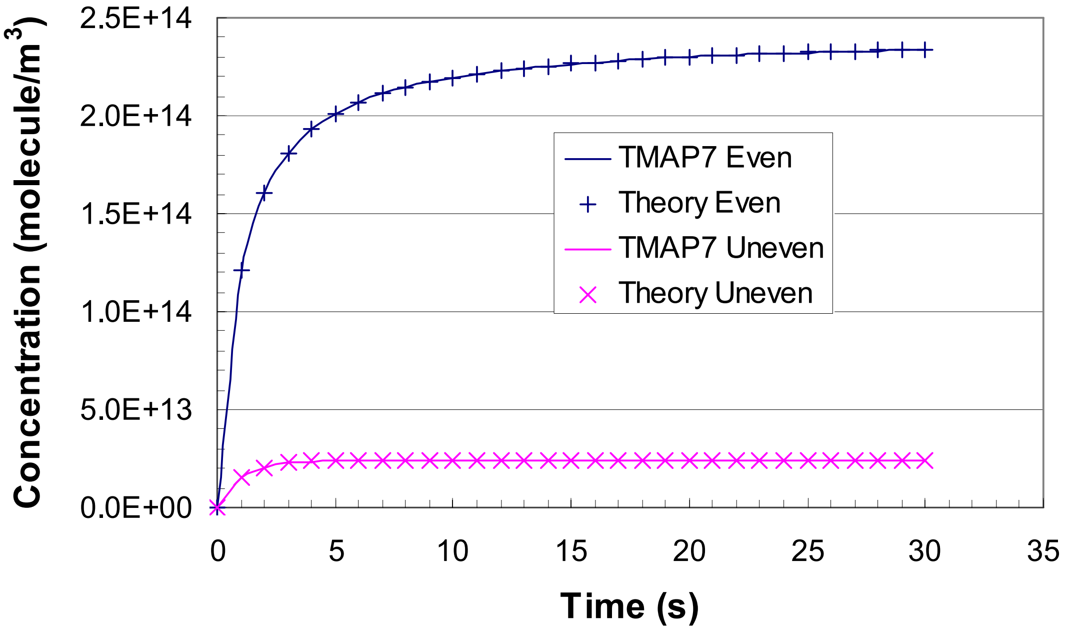

Figure 10. Production of [AB] from [A] and [B] under assumptions of equal and unequal initial reactant concentrations (Val-1ga/Val-1gb).

2.7.2 Series Reactions (Val-1gc)

The third problem modeled is a set of reactions in series. The system was configured so that the enclosure initially contained only species [A]. At time $t \geq 0$, the reactions were allowed to proceed. The reactions that were modeled are

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \,. \tag{35}$$

The production rate for each species (negative means consumption) is given by

$$-r_A' = k_1 C_A \tag{36}$$

$$r_B' = k_1 C_A - k_2 C_B \tag{37}$$

$$r_C' = k_2 C_B \tag{38}$$

Fogler[12] gives the concentrations of [A] and [B] as

$$C_A = C_{A_o} \exp(-k_1 t) \tag{39}$$

$$C_B = k_1 C_{A_o} \left(\frac{\exp(-k_1 t) - \exp(-k_2 t)}{k_2 - k_1} \right) \tag{40}$$

where

t = time (sec),

C_{A_o} = initial concentration of [A], (2.415×10^{14} atoms/m^3).

k_1 = rate constant of reaction 1 (0.0125 s^{-1})

k_2 = rate constant of reaction 2 (0.0025 s^{-1}).

The concentration of [C] was found by applying a mass balance over the system. From the stoichiometry of this reaction it was found that

$$C_C = C_{A_o} - C_A - C_B . \tag{41}$$

The concentration values of Equations (39), (40), and(41) were obtained using Microsoft Excel™. These numbers, converted to Pa were then compared with the pressure values obtained from TMAP7. The variance for the pressures of species A and B are less than 0.2% for all time. The variance of species C, begins at around 10%, but continually decreases as the problem time increases. The variance falls below 0.2 % at time, t = 34 sec. The value is initially high because of the division by a small number in Equation (6). The comparisons for this problem are listed in Table 16. A graphical representation is shown in Figure 11.

Table 16. Pressure of species in a series reaction.

Time	Conc [A]	Theory [A]	Variance A	Conc [B]	Theory [B]	Varianc B	Conc [C]	Theory [C]	Varianc C
0	1.00E-06	1.00E-06	0.00000	0.00E+00	0.00E+00	0.00000	0.00E+00	0.00E+00	0.00000
50	5.35E-07	5.35E-07	0.00039	4.34E-07	4.34E-07	-0.00056	3.07E-08	3.07E-08	0.00117
100	87E-07	2.87E-07	0.00082	6.15E-07	6.15E-07	-0.00042	9.81E-08	9.81E-08	0.00022
150	1.54E-07	1.53E-07	0.00121	6.67E-07	6.67E-07	-0.00028	1.79E-07	1.79E-07	0.00002
200	8.22E-08	8.21E-08	0.00166	6.55E-07	6.56E-07	-0.00016	2.62E-07	2.62E-07	-0.00011
250	4.40E-08	4.39E-08	0.00210	6.14E-07	6.14E-07	-0.00007	3.42E-07	3.42E-07	-0.00014
300	2.36E-08	2.35E-08	0.00252	5.61E-07	5.61E-07	0.00000	4.15E-07	4.15E-07	-0.00015
350	1.26E-08	1.26E-08	0.00293	5.05E-07	5.05E-07	0.00007	4.82E-07	4.82E-07	-0.00014
400	6.76E-09	6.74E-09	0.00339	4.51E-07	4.51E-07	0.00012	5.42E-07	5.42E-07	-0.00014
450	3.62E-09	3.61E-09	0.00384	4.01E-07	4.01E-07	0.00016	5.95E-07	5.95E-07	-0.00013
500	1.94E-09	1.93E-09	0.00427	3.56E-07	3.56E-07	0.00020	6.42E-07	6.42E-07	-0.00013
550	1.04E-09	1.03E-09	0.00474	3.15E-07	3.15E-07	0.00023	6.84E-07	6.84E-07	-0.00012
600	5.56E-10	5.53E-10	0.00513	2.78E-07	2.78E-07	0.00025	7.21E-07	7.21E-07	-0.00010
650	2.98E-10	2.96E-10	0.00556	2.46E-07	2.46E-07	0.00029	7.54E-07	7.54E-07	-0.00010
700	1.59E-10	1.58E-10	0.00599	2.17E-07	2.17E-07	0.00033	7.83E-07	7.83E-07	-0.00009
750	8.54E-11	8.48E-11	0.00645	1.92E-07	1.92E-07	0.00033	8.08E-07	8.08E-07	-0.00008
800	4.57E-11	4.54E-11	0.00687	1.69E-07	1.69E-07	0.00034	8.31E-07	8.31E-07	-0.00007
850	2.45E-11	2.43E-11	0.00733	1.49E-07	1.49E-07	0.00040	8.51E-07	8.51E-07	-0.00006
900	1.31E-11	1.30E-11	0.00774	1.32E-07	1.32E-07	0.00043	8.68E-07	8.68E-07	-0.00006

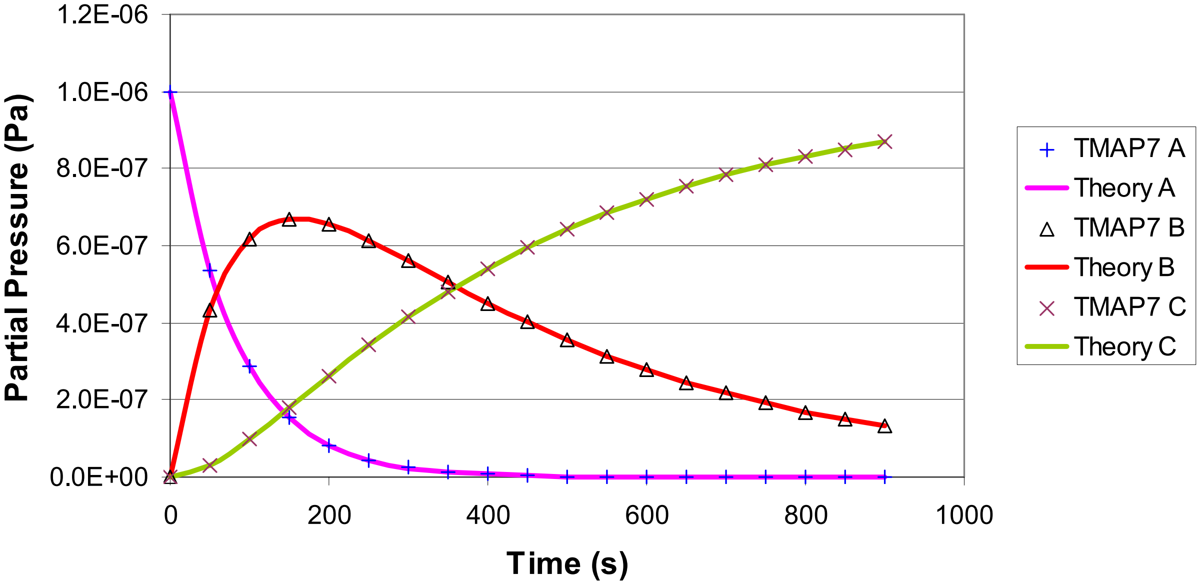

Figure 11. Partial pressures of species in series reaction (Val-1gc).

2.8 Problem 1h: Flow through Multiple Enclosures

These two problems are designed to model convective flow between enclosures. The first problem models three enclosures. The first enclosure is a *boundary* enclosure whose concentration is constant. A convective flow goes from enclosure 1, through enclosure 2, to enclosure 3, and then back to enclosure 1. In the second problem, two enclosures are pre-charged with different species and a convective flow is allowed to circulate the species between the two enclosures.

2.8.1 Three Enclosure Problem (Val-1ha)

A system of three enclosures is modeled with flow from 1, to 2, to 3, and back to 1. Since enclosure 1 is defined as a boundary enclosure, concentration is constant. This enclosure acts as a source and a sink. The flux, $\overline{j_i}$, of molecules entering into enclosure *i* is given by

$$\overline{j}_i = QC_{i-1} \tag{42}$$

where

Q = volumetric flow rate, common for all enclosures (0.1 $m^{3/}$sec)

C_{i-1} = concentration of gas molecules in enclosure i-1.

As the gas flows through the system, the number of atoms of the species of interest entering the 2nd and 3rd enclosures is greater than the number exiting. The concentration of that species in the enclosures rises towards the concentration in enclosure 1. The rate of change of the concentration of this species in the 2nd and 3rd enclosures can be modeled as follows

$$\frac{\partial P_2}{\partial t} = \frac{Q(P_1 - P_2)}{V_2}$$
$$\frac{\partial P_3}{\partial t} = \frac{Q(P_2 - P_3)}{V_3} \tag{43}$$

The solution of these simultaneous equations with the initial condition that $P_2 = P_3 = 0$ is

$$P_2 = P_1\left[1 - \exp\left(-\frac{Qt}{V_2}\right)\right] \tag{44}$$

and, if $V_2 = V_3$,

$$P_3 = P_1\left[1 - \left(1 + \frac{Qt}{V_2}\right)\exp\left(-\frac{Qt}{V_2}\right)\right] \tag{45}$$

Otherwise P_3 is given by

$$P_3 = P_1\left[1 - \frac{V_2}{V_2 - V_3}\exp\left(-\frac{Qt}{V_2}\right) + \frac{V_3}{V_2 - V_3}\exp\left(-\frac{Qt}{V_3}\right)\right] \tag{46}$$

In this problem, the following values were used to solve Equations (44) and (45),

$V_2 = V_3 = 1\ \mathrm{m}^3$,

$P_1 = 1.0\ Pa$,

$Q = 0.1\ \mathrm{m}^3/\mathrm{sec}$.

The values of Equations (44) and (45), were solved using Microsoft Excel™ and are compared with the values obtained from TMAP7 in Table 17 and Figure 12. The variance for both enclosures is less than 0.07% for all times.

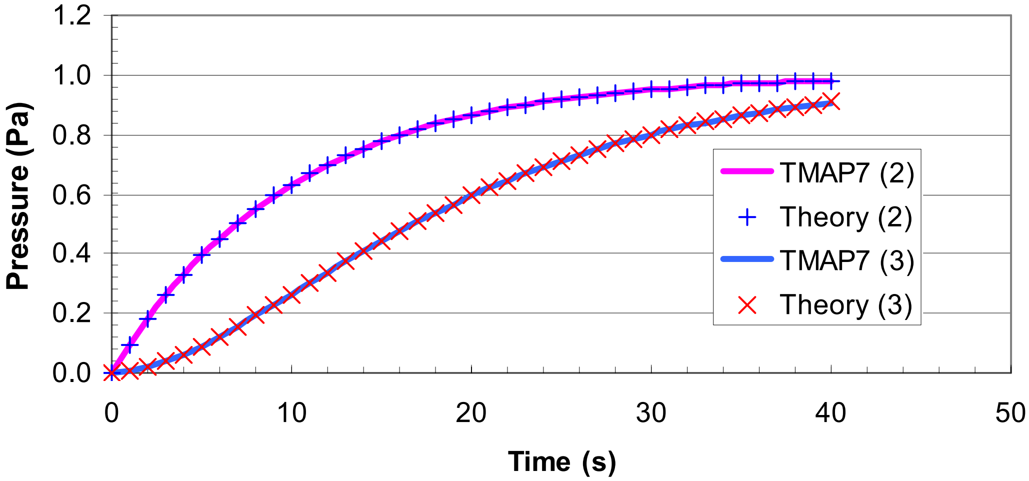

Figure 12. Pressure history of sequentially coupled enclosures (Val-1ha).

Table 17. Concentration profiles of enclosures 2 and 3 with convective flow.

	Enclosure (2)			Enclosure (3)		
Time (s)	TMAP7	Theory	Variance	TMAP7	Theory	Variance
0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1	0.09514	0.09516	-0.00022	0.00468	0.00468	0.00068
2	0.18123	0.18127	-0.00022	0.01753	0.01752	0.00022
3	0.25915	0.25918	-0.00012	0.03694	0.03694	0.00018
4	0.32965	0.32968	-0.00009	0.06156	0.06155	0.00016
5	0.39344	0.39347	-0.00007	0.09022	0.09020	0.00016
6	0.45112	0.45119	-0.00015	0.12190	0.12190	-0.00001
7	0.50330	0.50341	-0.00023	0.15577	0.15580	-0.00022
8	0.55051	0.55067	-0.00029	0.19114	0.19121	-0.00035
9	0.59324	0.59343	-0.00032	0.22741	0.22752	-0.00047
10	0.63191	0.63212	-0.00033	0.26410	0.26424	-0.00053
11	0.66690	0.66713	-0.00034	0.30080	0.30097	-0.00057
12	0.69856	0.69881	-0.00035	0.33717	0.33737	-0.00060
13	0.72721	0.72747	-0.00035	0.37294	0.37318	-0.00063
14	0.75321	0.75340	-0.00026	0.40801	0.40817	-0.00039
15	0.77674	0.77687	-0.00017	0.44210	0.44217	-0.00017
16	0.79802	0.79810	-0.00010	0.47506	0.47507	-0.00002
17	0.81727	0.81732	-0.00006	0.50682	0.50675	0.00013
18	0.83468	0.83470	-0.00003	0.53729	0.53716	0.00024
19	0.85044	0.85043	0.00001	0.56643	0.56625	0.00032
20	0.86469	0.86466	0.00003	0.59422	0.59399	0.00038
21	0.87758	0.87754	0.00004	0.62065	0.62039	0.00043
22	0.88924	0.88920	0.00005	0.64573	0.64543	0.00046
23	0.89979	0.89974	0.00005	0.66948	0.66915	0.00050
24	0.90934	0.90928	0.00006	0.69192	0.69156	0.00052
25	0.91797	0.91792	0.00006	0.71308	0.71270	0.00053
26	0.92571	0.92573	-0.00002	0.73283	0.73262	0.00029
27	0.93271	0.93279	-0.00009	0.75138	0.75134	0.00005
28	0.93905	0.93919	-0.00015	0.76881	0.76892	-0.00015
29	0.94479	0.94498	-0.00020	0.78517	0.78541	-0.00030
30	0.94999	0.95021	-0.00023	0.80049	0.80085	-0.00045
31	0.95470	0.95495	-0.00026	0.81484	0.81530	-0.00056
32	0.95896	0.95924	-0.00029	0.82825	0.82880	-0.00066
33	0.96283	0.96312	-0.00030	0.84078	0.84140	-0.00074
34	0.96632	0.96663	-0.00032	0.85248	0.85316	-0.00079
35	0.96949	0.96980	-0.00032	0.86338	0.86411	-0.00085
36	0.97236	0.97268	-0.00033	0.87354	0.87431	-0.00088
37	0.97495	0.97528	-0.00033	0.88300	0.88380	-0.00090
38	0.97730	0.97763	-0.00034	0.89180	0.89262	-0.00092
39	0.97943	0.97976	-0.00033	0.89997	0.90081	-0.00094
40	0.98140	0.98168	-0.00029	0.90772	0.90842	-0.00077

2.8.2 Equilibrating Enclosures (Val-1hb)

The second flow problem is setup as a system of two enclosures with flow from enclosures 1 to 2, and 2 to 1. Enclosure 1 is pre-charged with tritium and enclosure 2 is pre-charged with deuterium. The concentration change rates for this system are given by the following for species 't$_2$'

$$\begin{aligned} \frac{dC_{T_1}}{dt} &= \frac{Q}{V}\left(C_{T_2} - C_{T_1}\right) \\ \frac{dC_{T_2}}{dt} &= \frac{Q}{V}\left(C_{T_1} - C_{T_2}\right) \end{aligned} \tag{47}$$

and for species 'd$_2$'

$$\begin{aligned} \frac{dC_{D_1}}{dt} &= \frac{Q}{V}\left(C_{D_2} - C_{D_1}\right) \\ \frac{dC_{D_2}}{dt} &= \frac{Q}{V}\left(C_{D_1} - C_{D_2}\right) \end{aligned} \tag{48}$$

where

Q = volumetric flow (m^3/s)

V = volume (m^3)

C_{T_i} = concentration of tritium in Enclosure *i*

C_{D_i} = concentration of deuterium in Enclosure *i*

A mass balance on the system, gives a relationship between the concentration of species in Enclosure 1 and Enclosure 2. This can be seen in Equation (49).

$$C_{T_2}^{n} = C_{T_o} - C_{T_n}^{1} \tag{49}$$

Now by substituting Equation (49) into the first of equations (47), the solution is given by

$$C_{T_1} = C_T^S + \left(C_{T_1}^o - C_T^S\right)\exp\left(-\frac{2Q}{V}t\right) \tag{50}$$

where

$C_{T_i}^o$ = initial concentration of tritium in Enclosure 1,

C_T^S = Total concentration of tritium in system.

It is recognized that for the same initial starting conditions for deuterium, except different initial pressures (1 Pa in enclosure 2 and 0 Pa in enclosure 1), the following will be true

$$\begin{aligned} C_{D_2} &= C_{T_1} \\ C_{D_1} &= C_{T_2} \end{aligned} \tag{51}$$

Equation (50) was solved in Microsoft Excel™, substituting pressures for concentrations, and compared with the values obtained from TMAP7. These values are listed in Table 18. Concentrations of deuterium in each of the enclosures are shown graphically in Figure 13.

Table 18. Concentration of tritium in recirculating convective flow between two enclosures (Val-1hb).

	Enclosure 1			**Enclosure 2**		
Time (s)	**TMAP7**	**Theory**	**Variance**	**TMAP7**	**Theory**	**Variance**
0	1.0000E+00	1.0000E+00	0.00000	0.0000E+00	0.0000E+00	0
1	9.0937E-01	9.0937E-01	0.00001	9.0613E-02	9.0635E-02	-0.00024
2	8.3516E-01	8.3516E-01	0.00000	1.6482E-01	1.6484E-01	-0.00012
3	7.7443E-01	7.7441E-01	0.00003	2.2554E-01	2.2559E-01	-0.00024
4	7.2472E-01	7.2466E-01	0.00008	2.7524E-01	2.7534E-01	-0.00035
5	6.8402E-01	6.8394E-01	0.00012	3.1594E-01	3.1606E-01	-0.00038
6	6.5065E-01	6.5060E-01	0.00008	3.4930E-01	3.4940E-01	-0.00029
7	6.2329E-01	6.2330E-01	-0.00001	3.7666E-01	3.7670E-01	-0.00011
8	6.0089E-01	6.0095E-01	-0.00010	3.9905E-01	3.9905E-01	0.00000
9	5.8256E-01	5.8265E-01	-0.00015	4.1738E-01	4.1735E-01	0.00007
10	5.6757E-01	5.6767E-01	-0.00017	4.3237E-01	4.3233E-01	0.00009
11	5.5536E-01	5.5540E-01	-0.00007	4.4457E-01	4.4460E-01	-0.00006
12	5.4540E-01	5.4536E-01	0.00008	4.5453E-01	4.5464E-01	-0.00024
13	5.3723E-01	5.3714E-01	0.00017	4.6270E-01	4.6286E-01	-0.00035
14	5.3053E-01	5.3041E-01	0.00024	4.6940E-01	4.6959E-01	-0.00042
15	5.2504E-01	5.2489E-01	0.00028	4.7489E-01	4.7511E-01	-0.00046
16	5.2053E-01	5.2038E-01	0.00029	4.7940E-01	4.7962E-01	-0.00046
17	5.1672E-01	5.1669E-01	0.00006	4.8321E-01	4.8331E-01	-0.00021
18	5.1362E-01	5.1366E-01	-0.00008	4.8631E-01	4.8634E-01	-0.00006
19	5.1109E-01	5.1119E-01	-0.00019	4.8884E-01	4.8881E-01	0.00005
20	5.0903E-01	5.0916E-01	-0.00025	4.9090E-01	4.9084E-01	0.00012
21	5.0735E-01	5.0750E-01	-0.00029	4.9257E-01	4.9250E-01	0.00014
22	5.0603E-01	5.0614E-01	-0.00021	4.9390E-01	4.9386E-01	0.00008
23	5.0502E-01	5.0503E-01	-0.00001	4.9490E-01	4.9497E-01	-0.00015
24	5.0419E-01	5.0411E-01	0.00015	4.9574E-01	4.9589E-01	-0.00029
25	5.0349E-01	5.0337E-01	0.00024	4.9644E-01	4.9663E-01	-0.00038

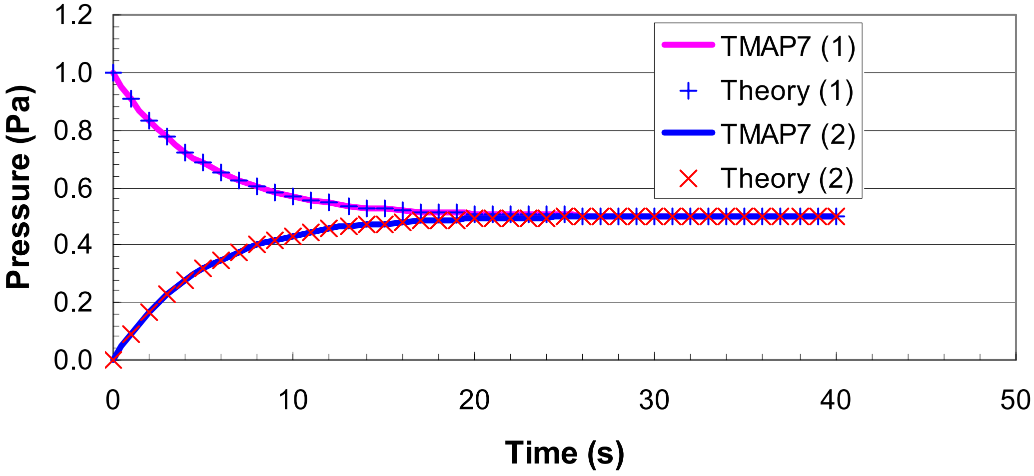

Figure 13. Partial pressure equilibration due to recirculating flow between two enclosures (Val-1hb).

2.9 Problem 1i: Species Equilibration on a Reactive Surface

When two species can react on a surface to form a third, it is possible to predict the rate at which equilibration between the species will occur. For example, consider the reaction between two isotopic species

$$A_2 + B_2 \Leftrightarrow 2AB \tag{52}$$

2.9.1 Ratedep Conditions

The expression (derived in Appendix A) for the rate of formation of AB, when the conversion rate at the surface is high, is given in terms of starting molecular partial pressures of A_2 and B_2 as

$$P_{AB} = \frac{2P_{A_2}^0 P_{B_2}^0}{\left(P_{A_2}^0 + P_{B_2}^0\right)}\left[1 - \exp\left(-\frac{SK_d kT}{V}t\right)\right] \tag{53}$$

Here

k = Boltzmann’s constant

T = Temperature

S = surface area where reactions take place

V = volume of enclosure adjacent to the surface

The molecular deposition and dissociation rate is often given by

$$K_d = \frac{1}{\sqrt{2\pi \ MkT}} \tag{54}$$

but it may be arbitrarily specified as well. The code was run for two initial starting conditions, equal and unequal starting pressures.

2.9.1.1 Equal Starting Pressures (Val-1ia)

The first case uses equal starting pressures of 1.0E+04 Pa of H_2 and D_2 and no *HD*. In this case K_d was specified to be 1.858E+24/$\sqrt{T}$. Temperature was 1,000 K, the surface area for reaction was a 5 cm x 5 cm square, and the enclosure volume was 1.0 m^3. Results are shown in Figure 14. Variance is less than 0.15% for all times.

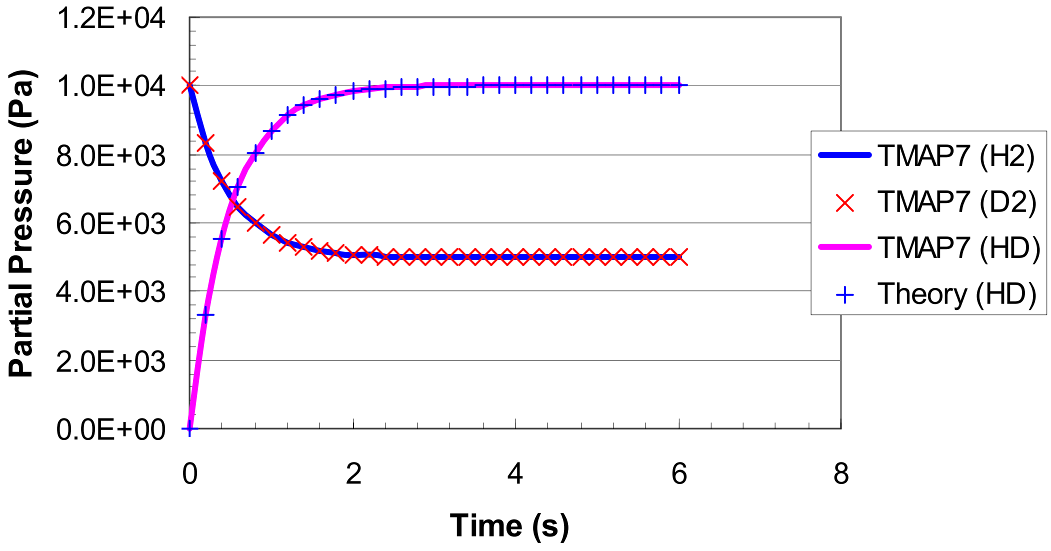

Figure 14. Species equilibration under *ratedep* boundary conditions for equal starting pressures of H_2 and D_2 (Val-1ia).

2.9.1.2 Unequal Starting Pressures (Val-1ib)

Unequal starting pressures were used by making the starting D_2 pressure in the previous problem 1.0E+05 Pa. Those results are shown in Figure 15. The variance with the time constant at 94% of theoretical is less than 0.2% for all times.

2.9.2 Surfdep Conditions

When surface process are governed by activation energies with dissociation and recombination considered explicitly, *surfdep* boundary conditions govern. As explained in Appendix A, the equation for transient pressure of HD given starting pressures of H_2 and D_2 is

$$P_{AB} = 2\frac{P^0_{A_2} P^0_{B_2}}{P^0_{A_2} + P^0_{B_2}}\left[1 - \exp\left(-\frac{t}{\tau}\right)\right] \tag{55}$$

where

$$\tau = \frac{V\left(\hat{K}_r + \hat{K}_b\right)}{SkT\,\hat{K}_d \hat{K}_b} \tag{56}$$

Now $\hat{K}_d$ is given by

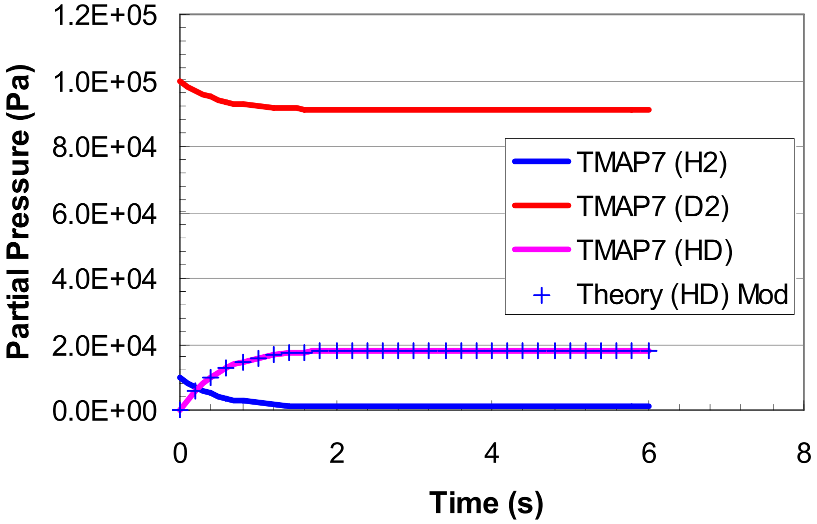

Figure 15. Species equilibration under *ratedep* boundary conditions for unequal starting pressures of H_2 and D_2 (Val-1ib).

$$\hat{K}_d = \frac{1}{\sqrt{2\pi\ MkT}} exp\left(-\frac{E_x}{kT}\right) \tag{57}$$

and recombination and dissociation coefficients are as given in Appendix A. For *surfdep* cases we used two different values of E_x but with equal starting pressures.

2.9.2.1 Low Barrier Energy, Equal Starting Pressures (Val-1ic)

The first of the *surfdep* cases uses equal starting pressures of 1.0E+04 Pa of H_2 and D_2 and no *HD*. In this case, E_x was specified to be 0.05 eV, E_c was -0.01 eV (both arbitrary values), and the dissociation energy was taken as zero, meaning that attempts at the Debye frequency all succeeded. Temperature was again1,000 K, the surface area for reaction was a 5 cm x 5 cm square, and the enclosure volume was 1.0 m^3. Results are shown in Figure 16. Agreement between theory and calculation is excellent, better than 0.08%. By comparison with Figures 14 and 15, it takes longer to come to steady state because of the finite delay the surface absorption barrier energy introduces.

2.9.2.2 Higher Barrier Energy, Equal Starting Pressures (Val-1id)

The second of the *surfdep* cases also uses equal starting pressures of 1.0E+04 Pa of H_2 and D_2 and no *HD*. In this case E_x was increased 0.2 eV, E_c was again -0.01 eV, and the dissociation energy was again taken as zero. Temperature was again1,000 K, the surface area for reaction was a 5 cm x 5 cm square, and the enclosure volume was 1.0 m^3. Results are shown in Figure 17. Agreement between theory and calculation is again excellent. It takes even longer to come to steady state because of the increased delay caused by the surface absorption barrier energy.

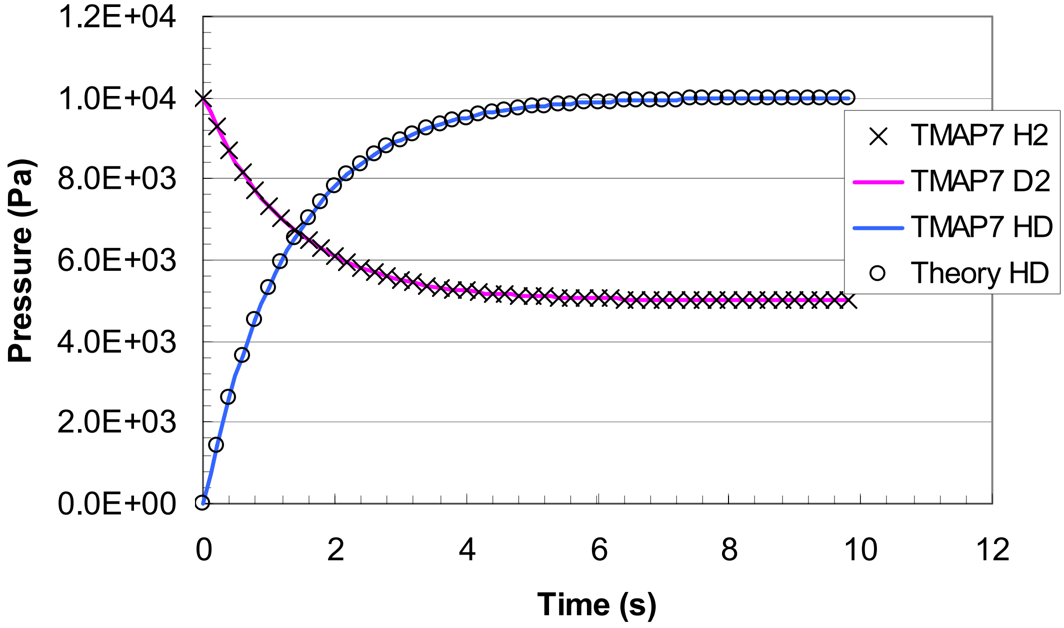

Figure 16. Species equilibrium under *surfdep* diffusion boundary conditions for equal starting pressures of H_2 and D_2 (val-1ic).

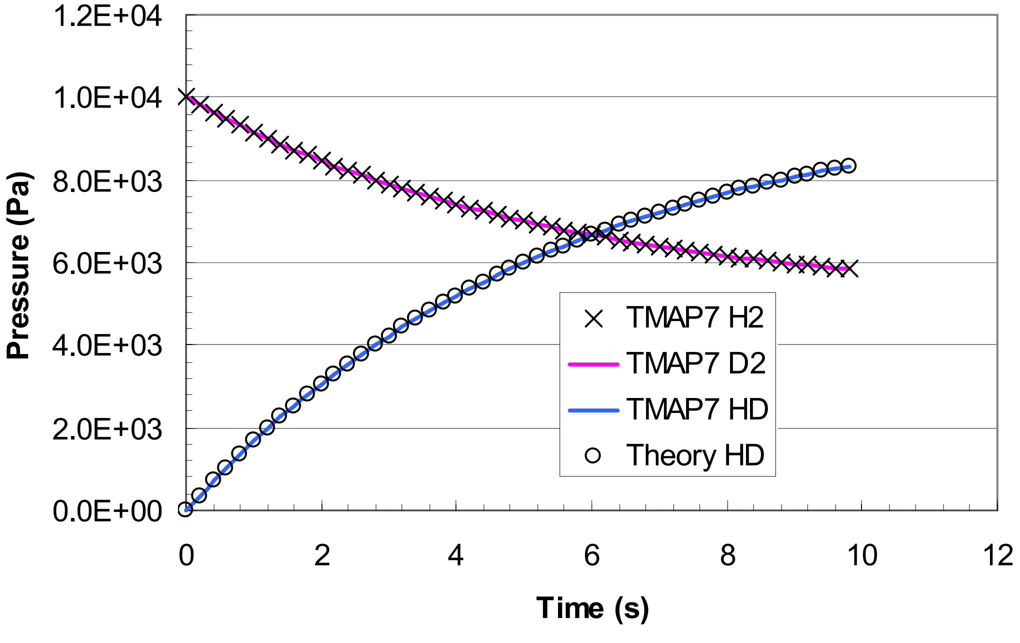

Figure 17. Species equilibration with 0.2 eV surface adsorption energy under *surfdep* diffusion boundary conditions.

2.9.3 Lawdep Conditions(Val-1ie, Val-1if)

This time the same problem is solved using *lawdep* diffusion boundary conditions.

2.9.3.1 Equal Starting Pressures (Val-1ie)

The first of the *lawdep* cases uses equal starting pressures of 1.0E+04 Pa of H_2 and D_2 and no *HD*. Once again, the enclosure volume is 1 m^3, and the reactive metal surface area is 25 cm^2. The solubility used was a simple constant, 1.0E+24 atom/m^3-$Pa^{1/2}$. The results are shown in Figure 18.

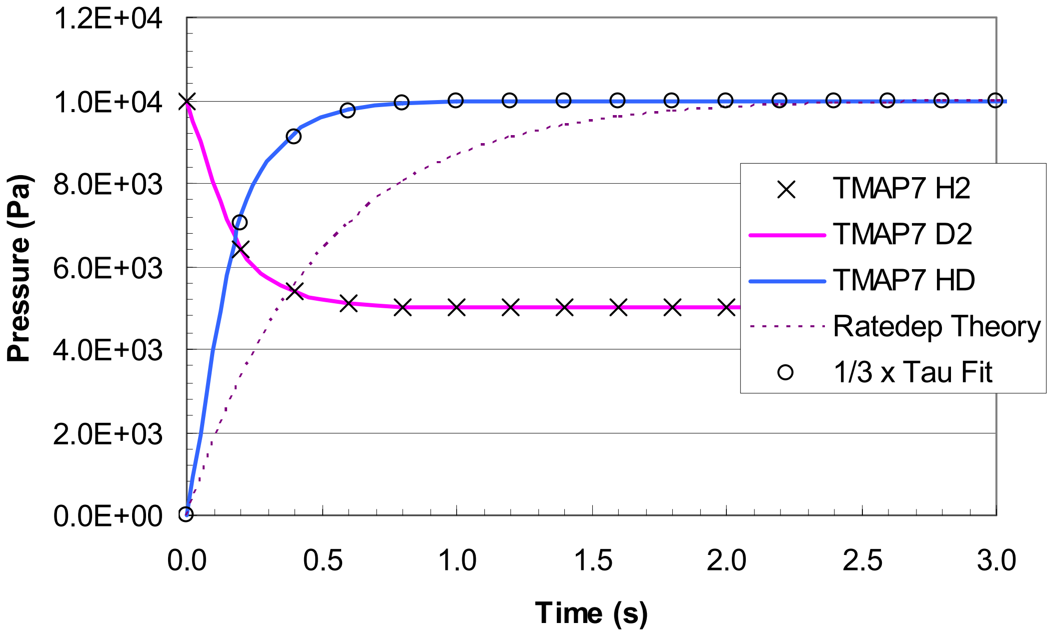

Figure 18. Species equilibration under *lawdep* conditions for equal starting pressures.

Lawdep diffusion boundary conditions for this problem are discussed in Appendix A. The rise in the *HD* pressure is a non-linear function, which is approximated at early times by a saturating exponential similar to the *ratedep* theory. There is also a surprisingly good fit achieved by calculating the time constant as 1/3 that given by the *ratedep* theory.

2.9.3.2 Unqual Starting Pressures (Val-1if)

The second *lawdep* case uses unequal starting pressures of 1.0E+04 Pa of H_2, 1.0E+05 Pa of D_2 and no *HD*. Once again, the enclosure volume is 1 m^3, and the reactive metal surface area is 25 cm^2. The solubility used was again 1.0E+24 atom/m^3-$Pa^{1/2}$. The results are shown in Figure 19. In this case, the best fit is achieved if the saturation time constant is reduced to 15% of the *ratedep* value.

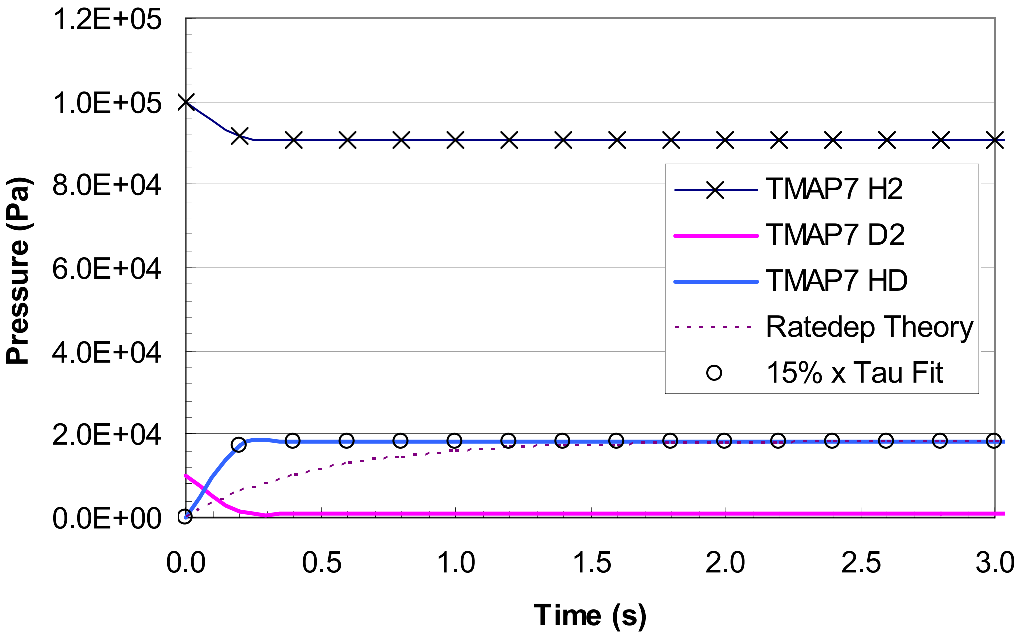

Figure 19. Species equilibrium under *lawdep* diffusion boundary conditions for uequal starting pressures of H_2 and D_2 (val-1if).

2.10 Problem 1j: Radioactive Decay

Two problems were run to demonstrate tritium decay, though any other isotope could have been chosen. The first is simple decay of mobile species in a slab. The second is decay of trapped atoms in a similar slab but with a distributed trap concentration.

2.10.1 Problem 1ja: Radioactive Decay of Mobile Tritium in a Slab (Val-1ja)

This model is employed to test the first order radioactive decay capabilities of TMAP7. The model assumes pre-charging of a slab with tritium. The tritium was uniformly distributed over the thickness of the slab. The tritium decays to ^{3}He with a half-life of 12.3232 years.

The concentrations of the two species are calculated. The concentration of T at any given time is given by

$$C_t = C_t^o \exp(-kt) \tag{58}$$

Applying a mass balance over the system, the concentration of helium is given by

$$C_{^3He} = C_t^o \left[1 - \exp(-kt)\right] \tag{59}$$

where

C_t^o = Initial concentration of tritium

k = rate constant (1.78241E-9 s^{-1})

t = time (sec).

The comparison between the TMAP7 result and Equations (58) and (59) for mobile tritium can be seen in Table 19. A graphical representation is given in Figure 20.

Table 19. Decay of mobile tritium to 3He (Val-1ja).

Time (yr)	TMAP7 T	Theory	Variance	TMAP7 He	Theory	Variance
0.00	1.5000	1.5000	0.00000	0.0000	0.0000	0.00000
1.10	1.4105	1.4105	-0.00003	0.0892	0.0895	-0.00333
2.19	1.3264	1.3264	-0.00001	0.1733	0.1736	-0.00165
3.29	1.2473	1.2473	0.00000	0.2524	0.2527	-0.00109
4.38	1.1729	1.1729	-0.00001	0.3268	0.3271	-0.00084
5.48	1.1030	1.1030	0.00003	0.3968	0.3970	-0.00065
6.57	1.0372	1.0372	0.00002	0.4626	0.4628	-0.00054
7.67	0.9754	0.9753	0.00005	0.5244	0.5247	-0.00047
8.76	0.9172	0.9172	0.00005	0.5826	0.5828	-0.00041
9.86	0.8625	0.8625	0.00005	0.6373	0.6375	-0.00035
10.95	0.8111	0.8110	0.00007	0.6888	0.6890	-0.00031
12.05	0.7627	0.7626	0.00007	0.7371	0.7374	-0.00029
13.14	0.7172	0.7172	0.00008	0.7826	0.7828	-0.00025
14.24	0.6745	0.6744	0.00009	0.8254	0.8256	-0.00023
15.33	0.6342	0.6342	0.00010	0.8656	0.8658	-0.00022
16.43	0.5964	0.5963	0.00009	0.9035	0.9037	-0.00020
17.52	0.5608	0.5608	0.00011	0.9391	0.9392	-0.00018
18.62	0.5274	0.5273	0.00010	0.9725	0.9727	-0.00017
19.71	0.4959	0.4959	0.00011	1.0040	1.0041	-0.00011
20.81	0.4664	0.4663	0.00013	1.0335	1.0337	-0.00018
21.90	0.4386	0.4385	0.00012	1.0614	1.0615	-0.00010
23.00	0.4124	0.4123	0.00013	1.0875	1.0877	-0.00014
24.10	0.3878	0.3878	0.00014	1.1121	1.1122	-0.00013
25.19	0.3647	0.3646	0.00014	1.1352	1.1354	-0.00015
26.29	0.3429	0.3429	0.00014	1.1570	1.1571	-0.00010
27.38	0.3225	0.3224	0.00015	1.1775	1.1776	-0.00006
28.48	0.3033	0.3032	0.00016	1.1967	1.1968	-0.00008
29.57	0.2852	0.2851	0.00018	1.2148	1.2149	-0.00007
30.67	0.2682	0.2681	0.00017	1.2318	1.2319	-0.00007
31.76	0.2522	0.2521	0.00018	1.2478	1.2479	-0.00006
32.86	0.2371	0.2371	0.00018	1.2628	1.2629	-0.00009
33.95	0.2230	0.2229	0.00019	1.2770	1.2771	-0.00004
35.05	0.2097	0.2097	0.00019	1.2903	1.2903	-0.00004
36.14	0.1972	0.1971	0.00022	1.3028	1.3029	-0.00004
37.24	0.1854	0.1854	0.00022	1.3145	1.3146	-0.00008
38.33	0.1744	0.1743	0.00022	1.3256	1.3257	-0.00005
39.43	0.1640	0.1639	0.00022	1.3360	1.3361	-0.00005
40.52	0.1542	0.1542	0.00021	1.3458	1.3458	-0.00003
41.62	0.1450	0.1450	0.00025	1.3550	1.3550	-0.00003
42.71	0.1364	0.1363	0.00024	1.3636	1.3637	-0.00006
43.81	0.1282	0.1282	0.00025	1.3718	1.3718	-0.00001
44.90	0.1206	0.1205	0.00023	1.3794	1.3795	-0.00004

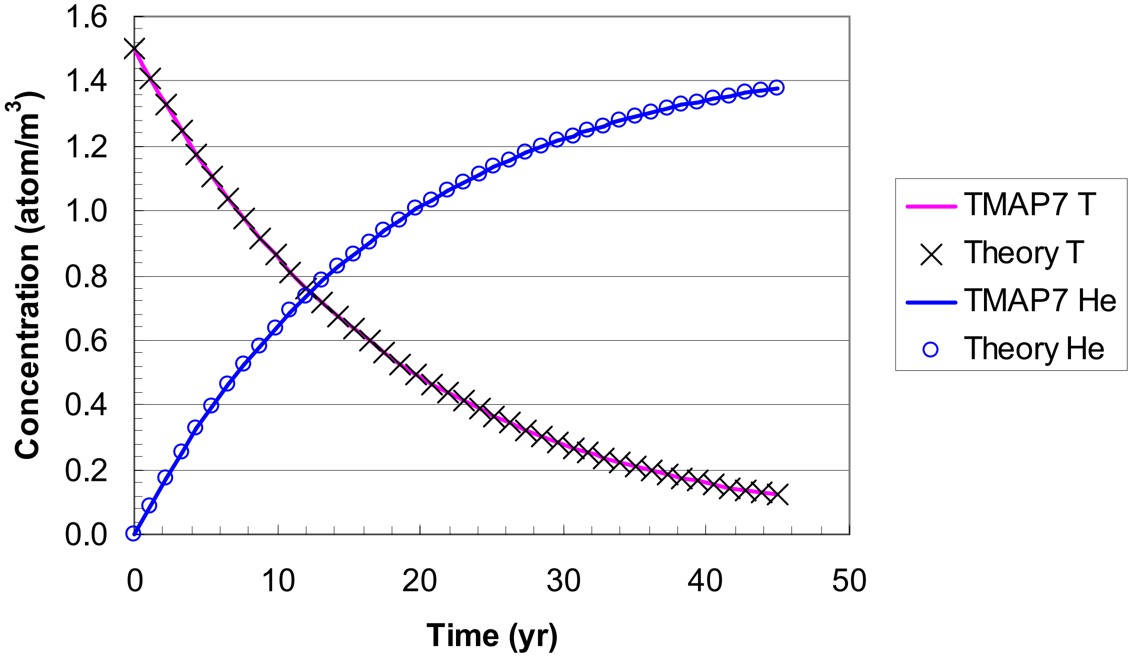

Figure 20. Decay of tritium and associated growth of ^{3}He in a diffusion segment (Val-1ja).

2.10.2 Problem 1jb: Decay of Tritium in a Distributed Trap (Val-1jb)

A further but more complex exercise was run for a slab in which nearly all of the tritium is trapped. A slab similar to that used in Problem 1ja was used here, but traps at 0.1% atom fraction and 4.2-eV trap energy were distributed in a normal distribution centered at the mid-plane of the slab. The traps were initially filled to 50% of trap concentration. The mobile atom concentration was only 1 atom/m^3 to begin with. This problem also demonstrates the utility of the pre-programmed distribution functions for certain parameters.

Figure 21 shows the depth profiles of initial trapped atoms of tritium, final trapped atoms of tritium after 45 years, and the distribution of He-3 at the end of that time. Note that because of zero diffusivity of the He-3, it has remained in the same profile as the trap concentration. The theoretical solution for this broadening under non-zero diffusivity is complex and is not presented here.

Figure 22 shows the total inventory of tritium in the trap as a function of time over the first 20 years of the decay period. It also shows the total helium inventory (atoms/m^2). The same precision as demonstrated in Problem 1ja was observed here.

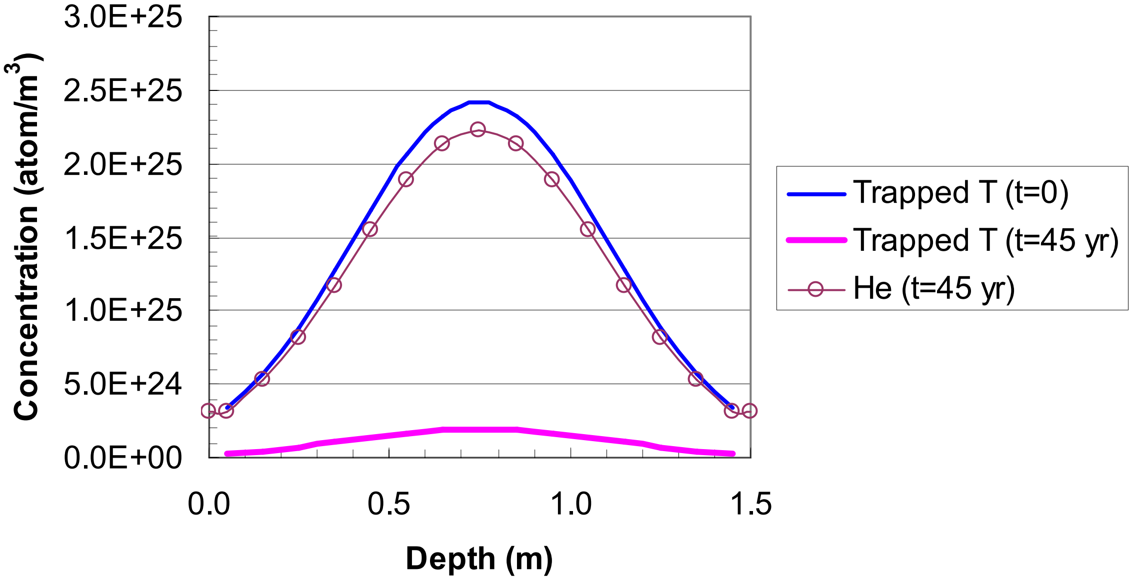

Figure 21. Concentration profiles of initially trapped tritium that decayed to ^{3}He over 45 years (Val-1jb).

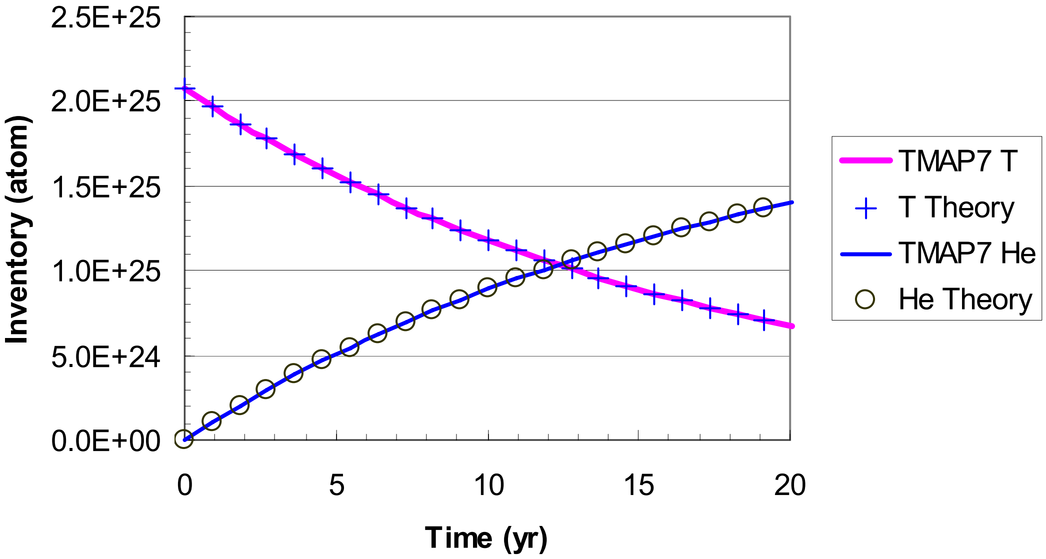

Figure 22. Concentration of trapped tritium and resulting He-3 over the first 20 years of dedcay.

2.11 Problem 1k: Enclosure Volumetric Source Rate

This problem involves two enclosures connected by a diffusive membrane with Sieverts law diffusion boundaries. Both enclosures have H_2, T_2, and HT. In one enclosure, there is an initial inventory of H_2 only and a constant volumetric source rate of T_2. The second enclosure begins initially empty.

This is a very difficult problem to solve analytically because it involves coupled non-linear partial differential equations with variable boundary conditions. However, the general behavior may be anticipated as follows. The H atoms should redistribute themselves in time such that they become distributed between the two enclosures in proportion to the volumes of the enclosures. The T atoms in the first enclosure will also redistribute. The constant rate of increase in the total number of T atoms in the system will not be equally distributed between the two enclosures because of the square root dependence on molecular partial pressure of transport from the first enclosure to the second. Initially, when the T_2 pressure in the first enclosure is small, the fraction transported to the second enclosure per unit time will be greater than it is later when the driving pressure is greater. Elements of this problem can be evaluated independently.

2.11.1 Simple Volumetric Source (Val-1ka)

The increase in pressure of T_2 molecules in the first enclosure can be observed by making the membrane between the two enclosures of *nonflow* type. Then the rate of pressure increase should be

$$\frac{dP_{T_2}}{dt} = \frac{S}{V} kT \tag{60}$$

where S is the volumetric source rate, V is the enclosure volume, k is the Boltzmann constant, and T is the enclosure temperature. Figure 23 shows the rise of the T_2 pressure in the first enclosure in response to a 1.0E+20 molecule/m^3-s T_2 source rate at a temperature of 500 K.

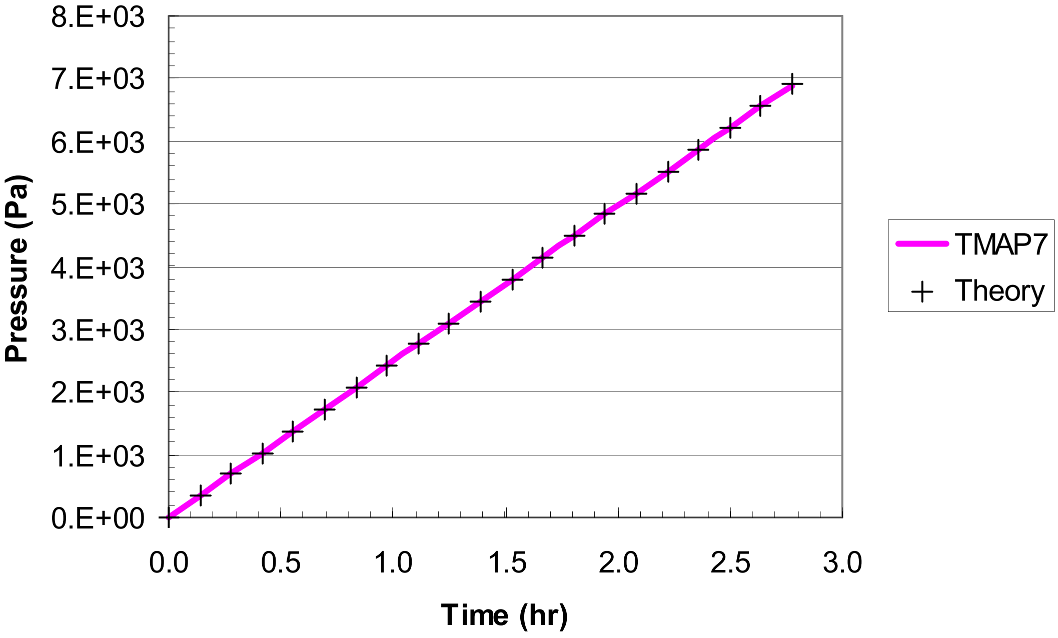

Figure 23. Rise of T_2 partial pressure in an enclosure with no loss pathways.

The variance is less than 0.018 % of its theoretical value.

2.11.2 Henry's Law Boundaries with No Volumetric Source (Val-1kb)

To see the equilibration of the system of the previous example without adding the complexity of a volumetric source, the membrane separating the two enclosures is changed to one with Henry's law diffusion boundaries and the volumetric source is removed. This means that there are *lawdep* boundary conditions, but the *pexp* parameter is 1.0 and there is no *espcomb* statement or isotopic adjustment.

In this case, the pressures of H_2 and T_2, the species having Henry's law solubility in the membrane separating the enclosures, will equilibrate over time. The heteronuclear species, HT, remains the same. The results are shown in Figure 24. Enclosure 2 has twice the volume of Enclosure 1, so the change in pressure there is only half the change in Enclosure 1.

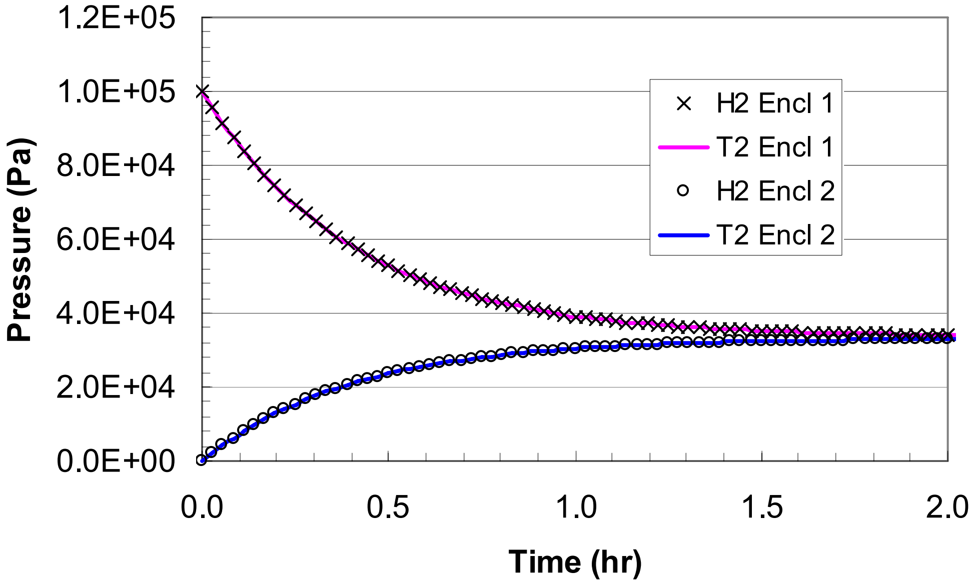

Figure 24. Equilibration of species pressures under Henry's law.

2.11.3 Sieverts' Law Boundaries with No Volumetric Source (Val-1kc)

The equilibration of the system of the previous example is now made more complex by changing the diffusion boundary condition from Henry's law to Sieverts' law, still without adding the complexity of a volumetric source, the membrane separating the two enclosures. Now all the species change in both enclosures, as shown in Figure 25.

In a very short time, the initial non-equilibrium distribution of isotopic species (1.0E+5 Pa H_2, 1.0E+5 Pa T_2, 1.0e-10 Pa HT) was corrected to the ratio 1:1:2. Also, the H and T diffusing through the membrane into the second enclosure distributed themselves in the same 1:1:2 ratio. The rate of approach to equilibrium between the enclosures is much slower than in the Henry's

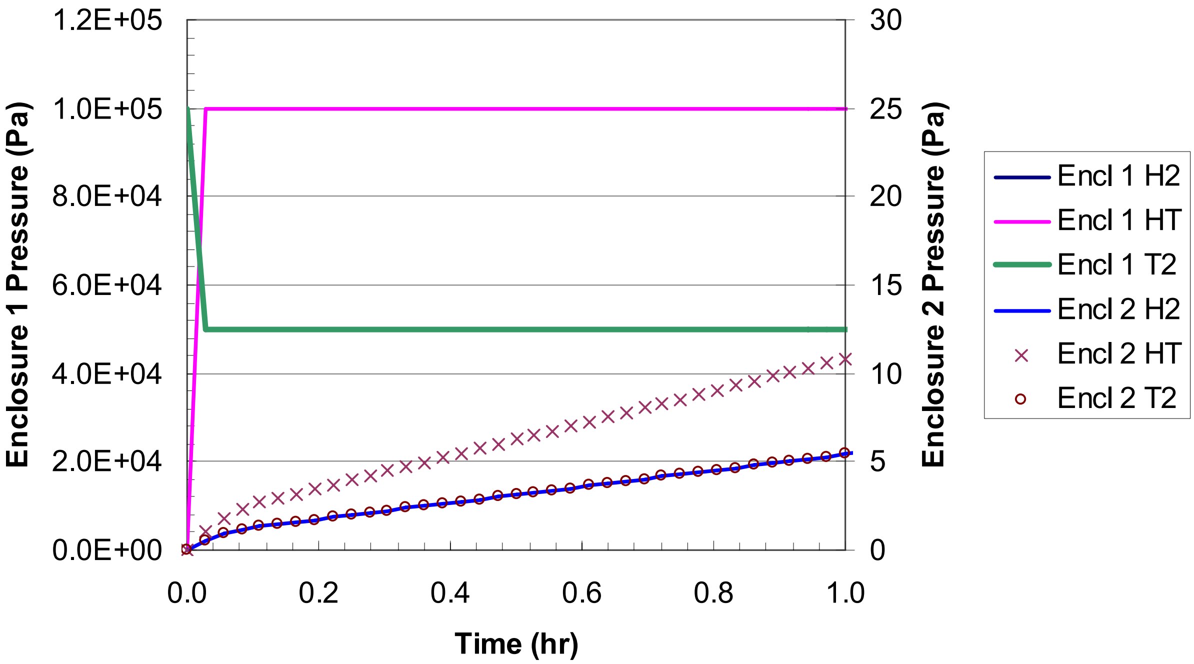

Figure 25. Sieverts' law diffusion boundary for equilibration between two enclosures.

law case even though the starting H_2 pressure, temperature, particle soolubility and diffusivity are the same. For the same surface species concentration, the starting pressure would have to be not 1.0E+05 Pa but 2.0E+10 Pa. The diffusing particles have only one H atom not two. It takes two diffusing particles to make a molecule on the downstream side, and only ½ of the molecules formed from the diffusing H become H_2. The initial transients in the first 0.1 hr in the second enclosure are diffusion transients as the atom concentration gradient is built up in the membrane separating the enclosures.

2.11.4 Sieverts' Law Boundaries with Volumetric Source (Val-1kd)

The final problem in this series adds to the previous problem the volumetric source rate of 10^{23} T_2/m^3-s. The results are plotted in Figure 26. The growth in the T_2 in each enclosure is evident even though the source was only in the first enclosure. Also note that in the first enclosure, the H_2 partial pressure decreases in time, not only by diffusion loss but also because with the increasing T_2 partial pressure, species equilibration pushes more and more of the H atoms into the HT form. The T_2 rise rate has an initial lag as some of the T_2 origninally in the first enclosure is transformed into HT. In the second enclosure, the rate of T_2 addition is rising in response to the increasing driving pressure from the other side of the membrane. H_2 in the second enclosure is approaching saturation due to declining H atom population in the first enclosure but mainly because witht he increasing prsence of T atoms in the second enclosure, more and more of the H atoms appear as HT there.

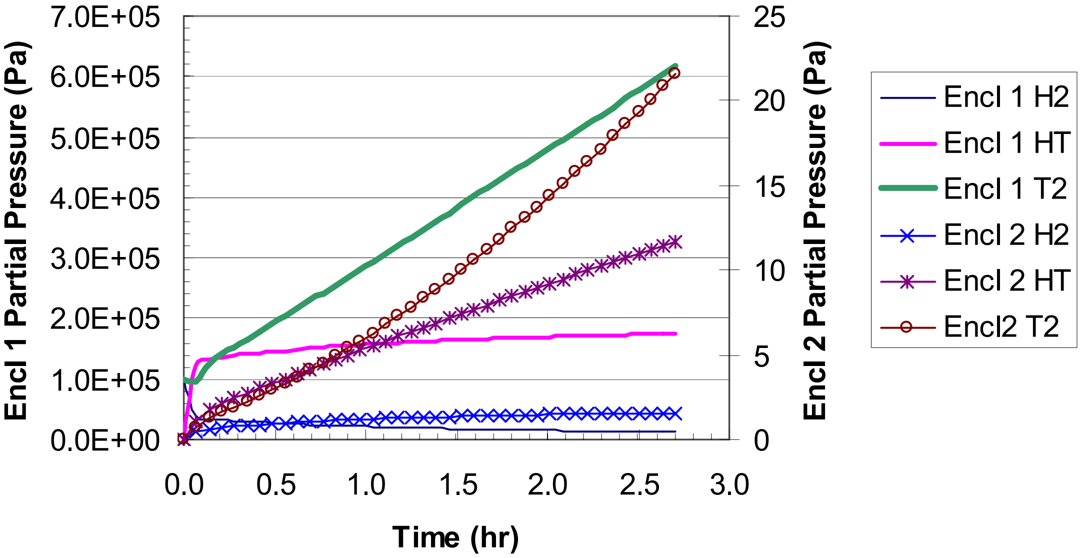

Figure 26. Equilibration between two enclosures with Sieverts' law boundaries and a volumetric source of T_2.

3.0 REPLICATING EXPERIMENTS

The second phase of code validation is the comparison of code results with actual experimental data. Published experiments together with their experimental data were selected for modeling. The first three of these are repeats from the verification and validation of TMAP4.[6]

3.1 Problem 2a: Ion Implantation Experiment (Val-2a)

This problem is the simulation of experimental results obtained at the INEL in 1985 and published.[13] 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 TMAP7 results and the experimental data are given in the publication. The TRIM code[14] was used to determine that the average implantation depth for the ions was 11-nm ± 5.4 nm. 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 modeling is that the cleanup of the upstream surface was modeled by a simple exponential in time rather than an integrated ion fluence which was interrupted twice during the actual experiment. The pressures upstream and downstream proved to be inconsequential; they could have been taken as zero and obtained essentially the same results. The plot of Figure 27 was generated. Actual experimental data are also shown on the

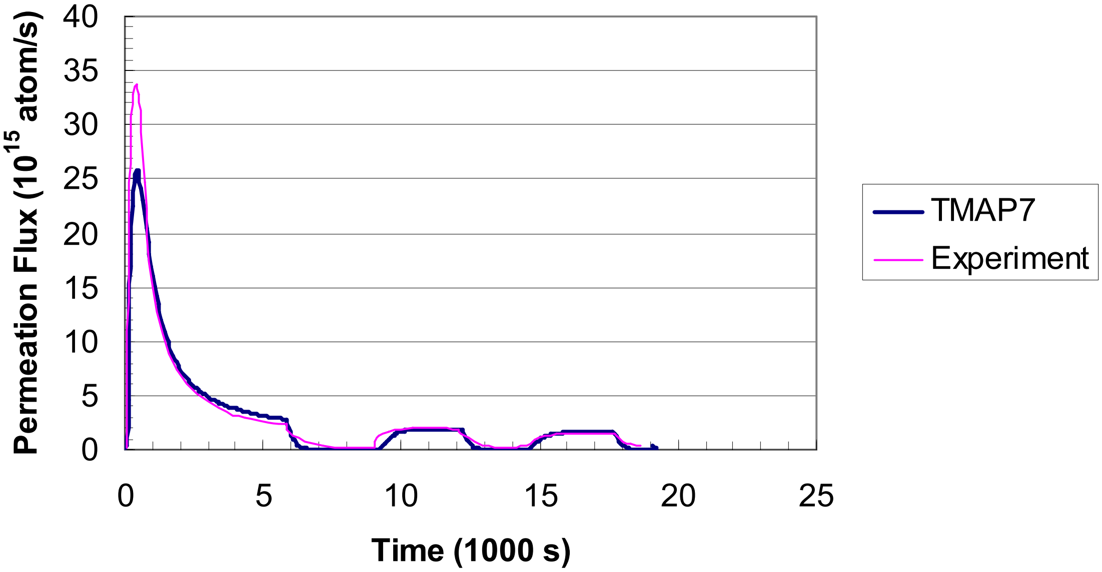

Figure 27. Plasma Driven Permeation of PCA (Val-2a)

figure. They are fairly closely approximated by the calculated permeation except at the very beginning. Some two-dimensional effects may have influenced the discrepancy there.

Results of this calculation using TMAP7 are a better fit than those obtained using TMAP4 and reported previously.

3.2 Problem 2b: Diffusion Experiment in Beryllium (Val-2ba, Val-2bb)

This problem is taken from work done by R. G. Macaulay-Newcombe at McMaster University.[15] 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 modeled here is that represented in Figure 12 (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 and 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 charging furnace, it was transferred in the air to a thermal desorption furnace where the temperature was increased from ambient (300 K) to 1,073 K at the rate of 3K/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 12 (a) of their paper are reproduced in Figure 16 here. 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 modeled using a two-segment model in TMAP7 with the segments linked. The first is the BeO film, which is modeled using 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 mid-plane. 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.,[16] 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. [17]. They made measurements on high-grade (99% pure) and extra-grade (99.8% pure). The values used here are those for high-grade beryllium, consistent with Dr. Macaulay-Newcombe's measurements of the purity of his samples.

Deuterium transport properties of the BeO are more challenging. First, it is not clear in what state the deuterium exists in the BeO. However, it has been observed[18] that an activation energy of -78 Kj.mole (exothermic solution) is evident for tritium coming out of neutron irradiated beryllium in work done 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.,[16] and by R. A. Causey, et al.,[19] among 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.[20] and in follow-up 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} $d/m^3Pa^{1/2}$. 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.[21]. 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 diffusivity, 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 diffusivity prefactor of the sintered material (7×10^{-5} m^2/sec) 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 Fowlers 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 have a complex distribution that results from first charging the sample and then discharging it during the cool down. 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 gives a good fit to the experimental data (Figure 28).

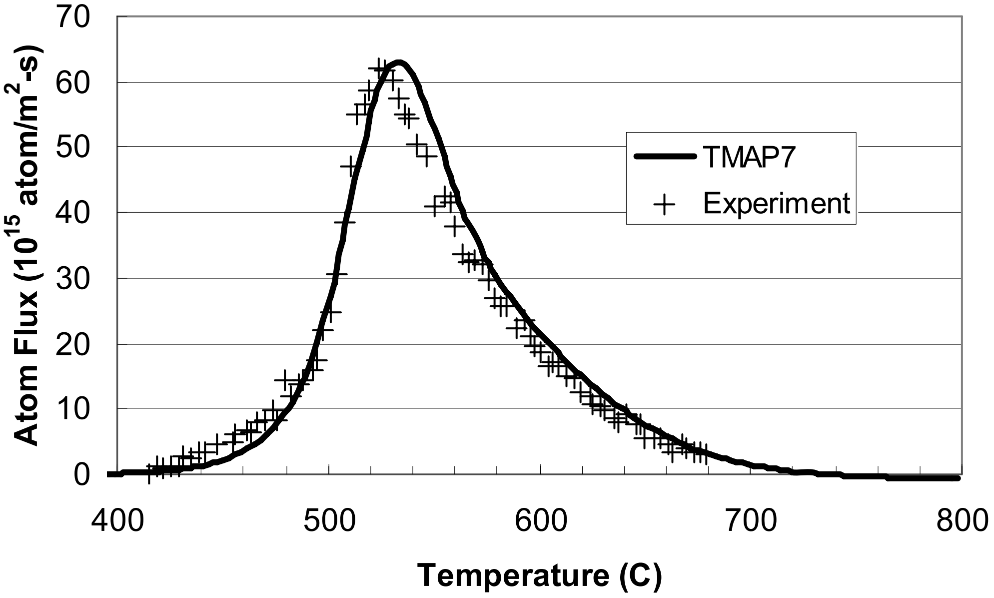

Figure 28. Thermal desorption test of beryllium (Val-2b).

The solid curve in Figure 28 is constructed from the extracted diffusion species surface flux data for the left side of thermseg/diffseg 1, where it is compared with the experimental data. Agreement is virtually identical with that found in the TMAP4 calculation for this problem.[6]

3.3 Problem 2c: Test Cell Release Experiment (Val-2c)

This is an experiment that involves multiple enclosures and chemical reactions. It was conducted at the Tritium Systems Test Assembly (TSTA) at Los Alamos National Laboratory and documented by Holland and Jalbert.[22] 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 through a secondary volume at the commencement of the experiment. Normally moist (20% R.H.) air was admitted to the chamber at the rate of 0.54m^3/hr constantly throughout the test. Of that, 0.06 m^3/hr was taken in through the secondary volume and exhausted through diagnostics including bubblers and an ion chamber. Samples of glycol taken form 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

$$T_2 + H_2O \Leftrightarrow HTO + HT \qquad (60)$$

$$HT + H_2O \Leftrightarrow HTO + H_2 \qquad (61)$$

took place within the exposure chamber, mainly as a consequence of the radioactivity of the tritium itself. Results of Holland and Jalbert are shown in their Figure 3 from the measurements of the resulting HTO concentration in the exposure chamber following a 10 Ci initial injection (effectively instantaneously) while purging with room air.

The TMAP7 Model for this experiment consists of four enclosures (1) the exposure chamber, (2) the room from which air is drawn, (3) the tritium waste treatment system (TWT) to which the exhaust gases are directed, and (4) the secondary enclosure through which T_2 as admitted. Enclosures (1) and (4) are treated as "functional" or chemically active. The other two are boundary enclosures. The paint on the inside of the exposure chamber is treated as a diffusive segment and non-flow conditions are employed 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 techniques for determining the constants and other information required to generate a model that gives reasonable results are slightly different from those given by Holland and Jalbert. The delay in reaching the peak value of HTO concentration in the bubbler water indicates that the T_2 was not injected as an initial condition as was previously modeled. Instead, the size of enclosure (4) was varied, maintaining 10 Ci as an initial T_2 inventory, until the delay in reaching the peak concentration matched the experimental data. That was found to be 0.15 m^3. It is not to be inferred that the actual volume was that size, but because of conversion to water and wall uptake and release conditions, it was an effective volume. Then the reaction rates were adjusted to give the appropriate peak in HTO concentration to match the data. It was assumed that the reaction rate stimulated by HTO was half that for the T_2. It was found that 2.0E-12 and 1.0E-12 m^3/Ci-s, just 1% of the values previously used, were appropriate for the T_2 and HTO, respectively. Finally, the solubility was adjusted to give the right decay rate for HTO concentration in the chamber. Solubility for elemental species was taken as 2.0E+19 molecule/m^3-Pa while the solubility for the oxides was 3.0E+24 molecule/m^3-Pa.

Data were calculated by TMAP7 for the HTO concentration in the exposure chamber, enclosure 2. A solid curve representing these data is compared in Figure 29 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 quite well at all times where the intercepts with the "average-value" line segments are at the correct times.

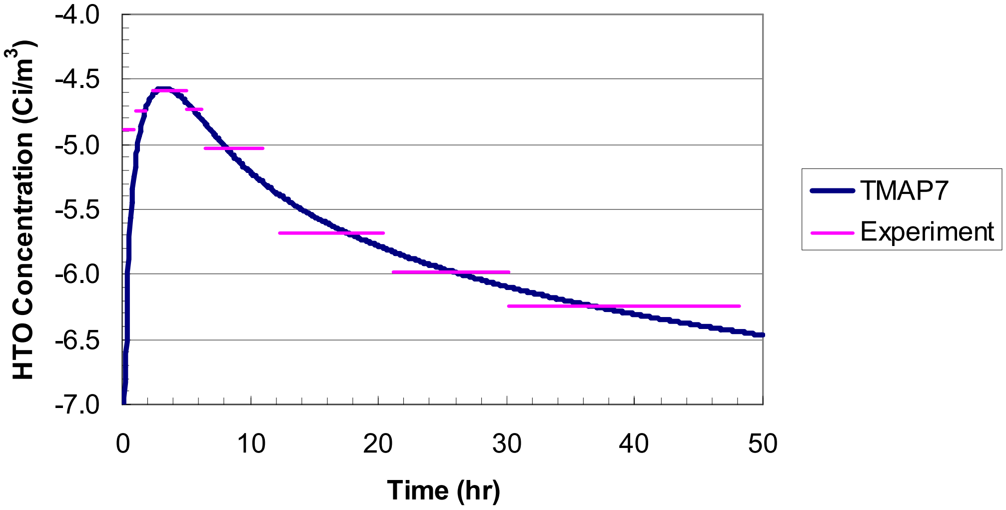

Figure 29. HTO Concentration in TSTA Exposure Chamber (Val-2c).

3.4 Problem 2d: Thermal Desorption Spectroscopy on Tungsten (Val-2d)

To exercise surface-law dependent diffusion boundary conditions and at the same time the multiple trapping capability, the experimental result of Hino et al.[23] was selected for approximation. In this experiment, H_3^+ was implanted at 5 keV and a flux of 1 x 10^{19} H/m^2s for 5,000 seconds into a polycrystalline tungsten foil 50 x 50 mm^2 and 0.1 mm thick at room temperature. Background pressure in the implantation chamber was 10^{-3} Pa while the implantation was going on and 10^{-5} Pa at other times. Following the implantation, the sample was subjected to thermal desorption spectroscopy by heating under vacuum at 50 K/min to 1,273 K and then held at that temperature for several minutes.

We modeled this system with TMAP7 using the structure of Figure 30. The implantation chamber (Encl 1) was assumed to have a volume of 0.1 m^3 and to be evacuated by a turbo-molecular vacuum pump. The test chamber was defined for this problem as a *functional* enclosure having a preprogrammed temperature of 300 K for 5,000 seconds followed by a ramp to 1,273 K at a ramp rate of 50 K/min. Gas leakage from the ion source was represented by a boundary enclosure with a pressure of 1E-03 Pa during implantation followed by 1E-05 Pa and flow to the implantation chamber at the vacuum pumping rate. Flow rate from the implantation chamber was taken to be 0.07 m^3/s on the basis of the stated pressure in the test chamber during implantation, given that nearly all implanted gas re-emerges during that time. The vacuum pump is represented by a *boundary* enclosure (Encl 2) held at 10^{-8} Pa.

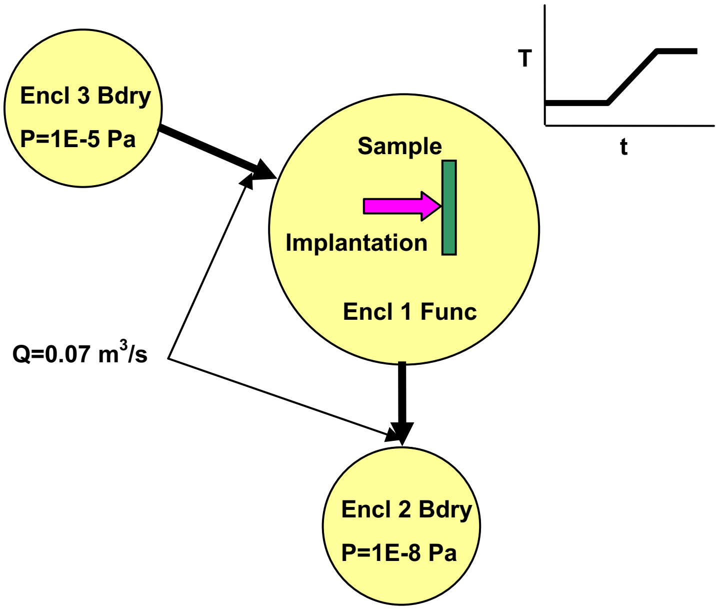

Figure 30. Schematic of system used to model experiments of Hino et al.[23]

On the basis of TRIM[2425] calculations, implantation was assumed to follow a normal distribution, peaking at 4.6 nm below the surface and having a scatter or characteristic half width of 3 nm. Implantation was active for 5000 seconds and then terminated. Hino et al.[23] also indicated implantation was at 4.6 nm.

The diffusion boundary condition employed was the *surfdep* or surface law dependent with the following parameter values

Atomic hydrogen, H

ν = DeBye frequency, 8.4E-12 (s^{-1})

E_c = surface binding energy, -0.8 (eV)

E_s = solution enthalpy, 1.04 (eV)

P_c = combination probability, 1.0 (to form H_2)

Surface hydrogen, H_2

ν_o = DeBye frequency, 8.4E-12 (s^{-1})

E_c = surface binding energy, -0.1 (eV)

E_x = surface barrier energy, 0.05 (eV)

M_m = molecular mass, 2.0 (amu)

P_c = formation probability, 1.0 (when H finds H)

For solubility of H in W, we use the value given by Frauenfelder.[26]

$$S = 1.778 \times 10^{24}\left(\frac{H}{m^3}\right) exp\left(-\frac{1.04\ eV}{RT}\right) \tag{62}$$

Diffusivity used for H through W was the normally accepted Frauenfelder value.[26]

$$D = 4.1 \times 10^{-7}\left(\frac{m^2}{s}\right) \exp\left(-\frac{0.39\ eV}{RT}\right) \tag{63}$$

H_2 was considered insoluble in W and therefore had no diffusivity through the bulk. However, the surface diffusivity was taken to be

$$D = 4.1 \times 10^{-7}\left(\frac{m^2}{s}\right) \exp\left(-\frac{0.1\ eV}{RT}\right) \tag{64}$$

Three traps were assumed in the sample. Trap concentrations and distributions were considered adjustable parameters while energies were determined by TDS peak temperatures. The first was assumed to be associated with implantation (damage and precipitation) and to be normally distributed with a peak at 4.6 nm and a characteristic width of 10 nm, consistent with the observations of Haasz et al.[27] that damage zone exceeds the implantation depth. Its trap energy was adjusted, based on the temperature of the first peak, to be 1.2 eV, and it was assumed to be 0.086 atom fraction at the peak. The second was a uniform trap, probably associated with dislocations and was assigned a trap release energy of 1.6 eV, typical of but slightly higher than that seen by Anderl et al.[28] Its concentration was adjusted to .0041 atom fraction. The third trap was also assumed to be uniformly distributed and to have a trapping energy of 3.1 eV, nearly the same as the deep trap seen by Frauenfleder[26] with a concentration of 2,000 appm. It was only marginally filled during the implantation because of the diffusive limitation to flow into the depth of the sample.

These values gave a peak surface flux averaged over both sides of the sample of 10^{18} H_2/m^2s at 500 seconds into TDS, to match the flux quoted by Hino et al. The experimental flux measurement was made using a residual gas analyzer, so the general background drift with temperature was probably due to an increasing source of atoms going into the gas phase as the heated region spread with time. For that reason, we have added to the results of the TMAP7 calculation a ramped signal peaking at 4.87×10^{17} $H_2/m^2.s$ during thermal desorption. The computed surface flux from the sample is shown together with the Hino data in Figure 31.

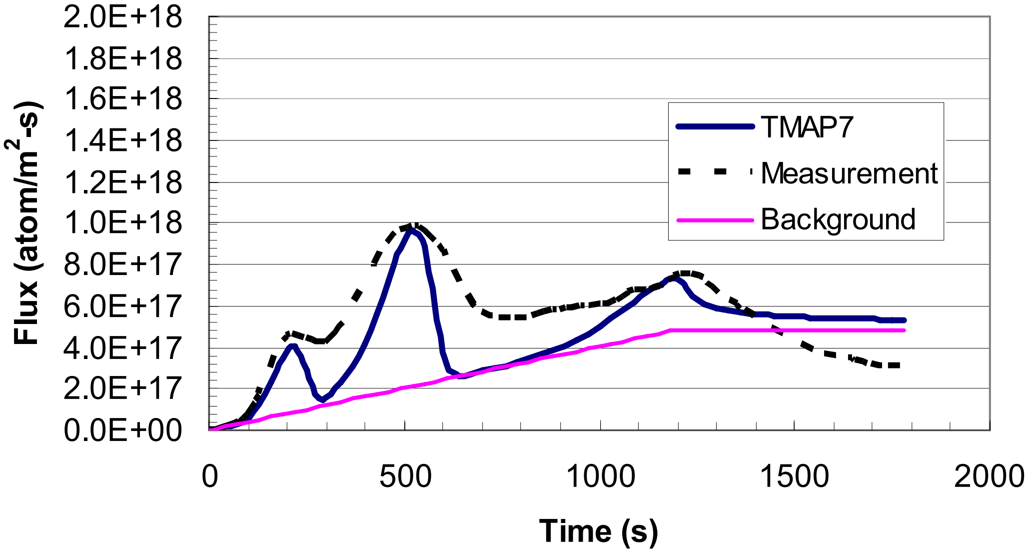

Figure 31. Comparison of calculated with experimental results for Hino's experiment with implantation and thermal desorption of tungsten (Val-2d).

The fit with the Hino et al. data is not exact because of several factors, the most prominent of which is probably the two-dimensionality of the experiment arising from beam non-uniformity and radial diffusion.[28] Actual trap energies are probably a little lower than the ones indicated above if the time lag caused by two-dimensionality is significant. Exchange of hydrogen with chamber surfaces, particularly the sample support structure, may also be a factor.

One reason the measured signal falls off while the computed one shown does not is that the source of additional atoms in the experiment may be an expanding area that grew more or less linearly while the sample was being heated but stopped growing and thus stopped emitting when the heating stopped.

3.5 Problem 2e. Co-permeation of H_2 and D_2 through Pd

This problem was selected to demonstrate a non-classical solution law boundary condition with molecular exchange as well as combined solution-law and recombination limited boundary conditions. It comes from work reported by Kizu et al.[29] on experiments in which H_2 and D_2

were allowed to permeate through thin Pd membranes either separately or together. The tests resulted in the formation of HD, both on the upstream side and on the downstream side of the membrane.

The experimental apparatus consisted of two vacuum chambers separated by a Pd membrane which was 1.8 x 10^{-4} m^2 in area and either 0.025 mm or 0.05 mm thick, depending on the test. The membrane was clamped on each side by a copper gasket, and it may reasonably be inferred that the only means of transfer of gas from one chamber to the other was by diffusion through the membrane. Temperatures in the membrane were controlled between 820 and 870 K by means of an electric resistance heater surrounding the membrane and a thermocouple touching the membrane. Gas was introduced into one of the chambers from regulated supply bottles at various compositions and pressures. Here, we refer to that chamber as the upstream chamber. The base pressure on both upstream and downstream chambers was maintained at less than 10^{-6} Pa by a combination of turbomolecular pump and rotary backing pump on each side. Pressure was indicated by an ion gage on each side, and downstream gas composition was measured with a quadrupole mass spectrometer. Flow rates through the membrane were determined by pressure increases in the downstream chamber at fixed pumping rate of 0.1 m^3/s.

The first tests reported were permeation tests of D_2 alone through membranes of each thickness. For the thinner membrane, tests were conducted at both 825 K and 865 K whereas the 0.05-mm membrane was tested only at 825 K. These were performed to calibrate the permeability of the membranes to hydrogen isotopes. Figure 32 shows their experimental data for permeation flux, $J(D_2)$, as a function of upstream D_2 pressure, $P(D_2)$.

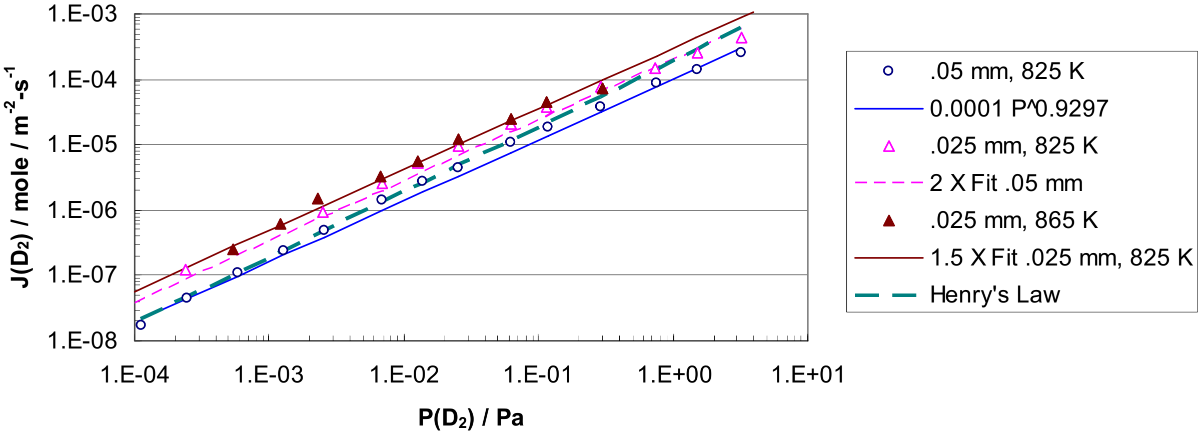

Figure 32. Permeability data of Kizu et al. for D_2 in Pd.

Also shown in Figure 32 are three "fit" lines and one showing first power dependence on D_2 pressure.. Kizu et al. observed that at low pressures the permeation flux is directly proportional to the upstream gas pressure. As pressure increases, the permeation flux falls off from that linear relationship and approaches a lower power dependence. Here, the fit to the 0.05-mm data (825 K) is made across the range of pressures measured, not just at the lower pressures where greater linearity is observed. The fit line to the 0.025-mm data (825 K) is not really a fit at all. It is simply the line from the 0.05-mm data multiplied by a factor of 2. It fits the data amazingly well, indicating that permeation through the membrane is diffusion-limited, not surface-limited. The fit line for the 865-K data has the same exponent (0.9297) as the previous two fit lines, but it is offset by a factor of 1.5 from the line through the 825-K data for the same 0.025-mm thickness. It does not fit the higher-pressure data as well as it does the low-pressure data, but it does suggest a permeability activation energy of 0.623 eV (7,234 K). The resulting equation for D_2 permeability in Pd is thus

$$J = \frac{2.042 \times 10^{-5}}{L} P^{0.9297} exp\left(-\frac{7234}{T}\right) \left(\frac{mole}{m^2 s}\right) \tag{65}$$

where

L = membrane thickness (m)

P = upstream pressure (Pa)

T = Temperature (K)

For the diffusion-limited regime, permeability is the product of solubility, S, and diffusivity, D, such that

$$J = \frac{C_0}{L} D = \frac{S\,P^{\nu}}{L} D = \frac{S_0\,P^{\nu} D_0}{L} \exp\left[-\frac{(E_d + E_s)}{kT}\right] \tag{66}$$

where E_d and E_s are the diffusion activation energy and solution enthalpy, respectively. Comparing Eqs. (65) and (66), we see that

$\nu = 0.9297$

$S_0 D_0 = 2.042 \times 10^{-5}$ (mole/m^2.s)

$E_d + E_s = 7{,}234\ k$ (J)

We can separate diffusivity and solubility by making use of the diffusivity of hydrogen in Pd given by Katz and Gulbransen[30] divided by $\sqrt{2}$ to account for isotopic effect on diffusivity

$$D_D = 2.636 \times 10^{-4} exp\left(-\frac{1315.8}{T}\right) \left(\frac{m^2}{s}\right) \tag{67}$$

That leaves

$$S = 0.07765\, exp\left(-\frac{5{,}918}{T}\right) \left(\frac{mole}{m^3 Pa^{\nu}}\right) = 9.355 \times 10^{22} exp\left(-\frac{5{,}918}{T}\right) \left(\frac{atom}{m^3 Pa^{\nu}}\right) \tag{68}$$

Next, we construct a model for TMAP7 simulation of this experiment. We consider two functional enclosures, each with an estimated volume of 0.005 m^3, separated by a diffusion segment of thickness L and area 1.8×10^{-4} m^2. This is illustrated in Figure 33.

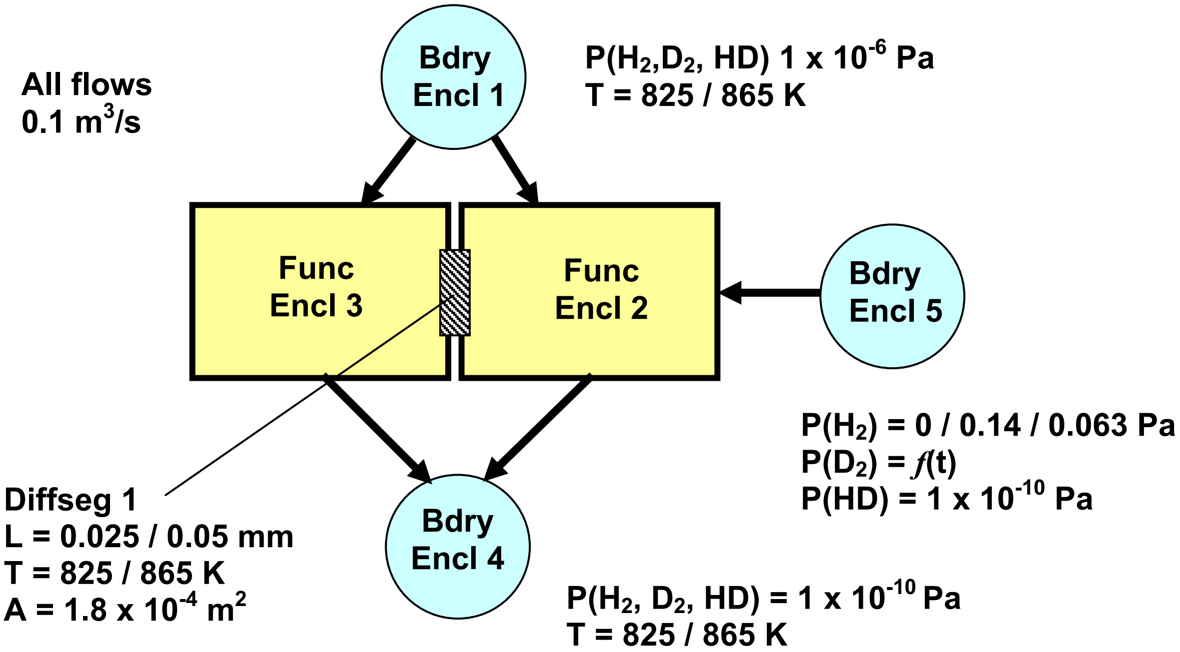

Figure 33. TMAP7 model of experimental system of Kizu et al.

Boundary enclosure 1 is the source of background pressure to the experimental system. Boundary enclosure 4 is the vacuum pumping system that provides a sink for all system flows. Boundary enclosure 5 is the gas feed to the upstream experimental chamber, functional enclosure 2. Depending on the experiment, the feed pressure of H_2 is 0, 0.14 Pa, or 0.063 Pa. Combined with the evacuation to boundary enclosure 4, this provides the upstream H_2 pressure for permeation. The D_2 pressure is a stepped function of time, one step corresponding to each of the data points in the data plots of Kizu et al. Steps are arbitrarily set at 100 s, but equilibrium is achieved in times much shorter than that. Effectively no HD is fed into the upstream experimental chamber, in keeping with the experimental setup given by Kizu et al. Rather, with either solution-law or recombination limited-boundary conditions for diffusion, HD is formed in accordance with the laws of chemical equilibrium. Likewise in the downstream chamber, functional enclosure 3, HD is formed together with H_2 and D_2 in chemical equilibrium from diffusing H and D.

We first replicate the calibration experiments shown in Figure 32 using input files Val-2ea.inp, Val-2eb.inp, and Val-2ec.inp for the three cases shown in Figure 32. Results are in Figure 34. The results are nearly identical with the approximations for the permeability in Figure 32.

In modeling the co-permeation of H and D, we first apply a *lawdep* boundary condition in which we apply H_2 through enclosure 5 at a constant pressure of 0.063 Pa and D_2 a pressures corresponding to the effective deuterium pressures, $P(D_2) + P(HD)/2$, given by Kizu et al. for their experiment on a 0.025-mm membrane (Val-2ed) at 870 K. The results of that computation arecompared with the experimental data in Figure 35.

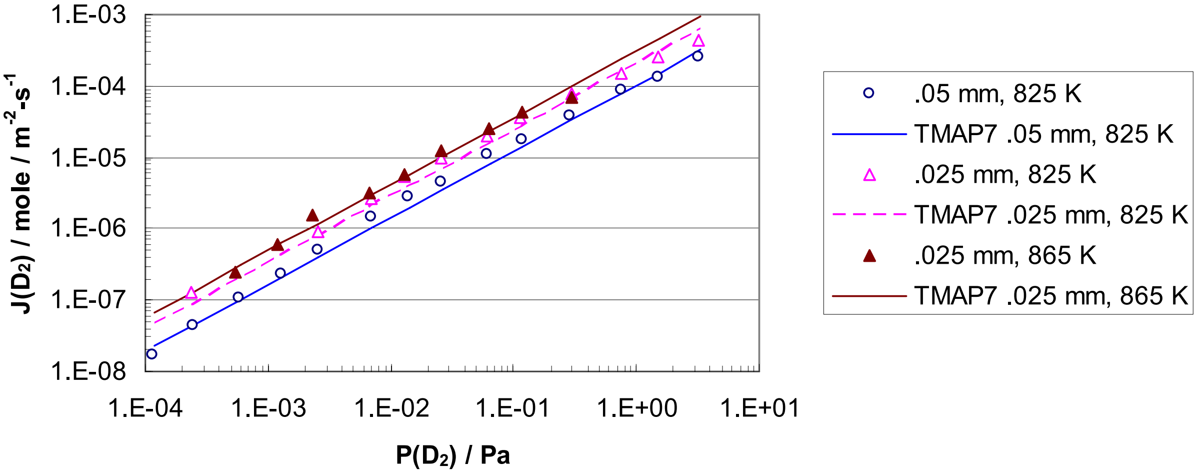

Figure 34. Comparison of TMAP7 permeation calculations with permeation data of Kizu et al. (Val-2ea, Val-2eb, Val-2ec).

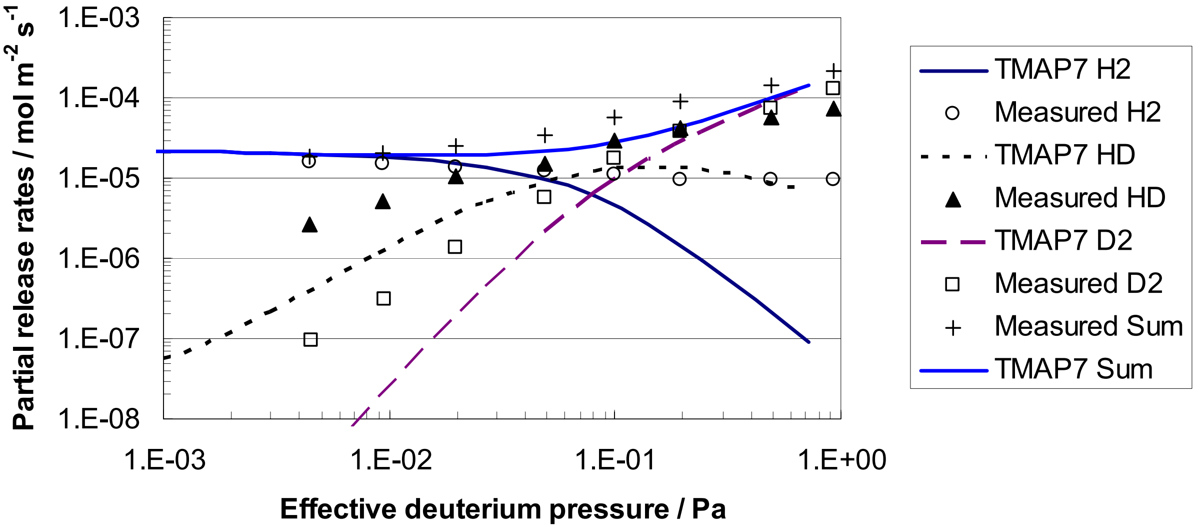

Figure 35. Comparison of TMAP7 results using a *lawdep* boundary condition on each side of the membrane with the experiment s of Kizu et al. (Val-2ed).

It is evident that while the H_2 release rates calculated at low pressures agree with the experimental data, they do not agree at higher pressures. D_2 release rates agree well at higher pressures but are substantially lower than measured at low pressures. The calculated HD release rates at all pressures follow log-mean theory for pressure equilibrium

$$P(HD) = 2\sqrt{P(H_2)P(D_2)} \tag{69}$$

but they do not agree with measurements, except they come closest at moderate deuterium pressure. The combined release rates agree well at upstream deuterium pressure extremes but not at intermedaite pressures where they are low by a factor of 3. Note that it is evident from the sketch provided by Kizu et al. of their experimental apparatus that there was no way to determine the individual species partial pressures in the upstream chamber during the experiment. Therefore, they used abscissa values based on equivalent deuterium pressure.

For additional perspective, we changed the diffusion boundary condition to the *ratedep* mode in which dissociation and recombination take place independently (Val-2ee). We use for the dissociation rate coefficient 0.0083 of the molecular arrival rate to the surface

$$K_d = \frac{1}{120\sqrt{2\pi MkT}} = \frac{2.1897\times 10^{22}}{\sqrt{MT}} \quad \left(\frac{molecule}{m^2 Pa}\right) \tag{70}$$

where *M* is the species molecular weight in amu. For the recombination coefficient, we use the relationship from Sieverts' law that

$$K_r = \frac{K_d}{S^2} = \frac{2.502\times 10^{-24}}{\sqrt{MT}} exp\left(\frac{11{,}836}{T}\right) \quad \left(\frac{m^4}{s}\right) \tag{71}$$

Here *S* is the solubility from Equation (68). The results from that computation are quite good except at high upstream deuterium pressures, as shown in Figure 36.

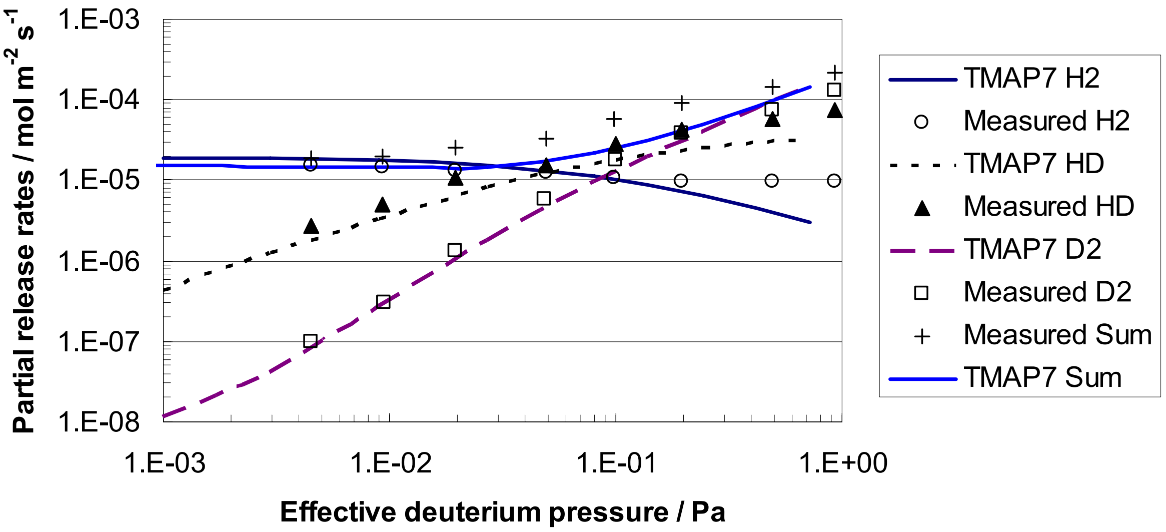

Figure 36. Comparison of TMAP7 calculation with simple *ratedep* boundary conditions with the values measured by Kizu et al. (Val-2ee).

Now, the fit for deuterium is excellent at all but the highest pressures. The agreement for H_2 is similar at low upstream deuterium pressures to that in Figure 35, but the model still under-predicts at higher pressures. Agreement for HD is excellent at low pressures, but it differs a little at higher pressures. Overall permeation rate is good at pressure extremes but it underpredicts at intermediate pressures.This is consistent with the mid-range departure of the fit for the deuterium data in Figure 34.

These results are consistent with the observations of Kizu et al. that permeation appears to be nearly first-order in P at low pressures but tends toward becoming proportional to $P^{1/2}$ as driving pressure increases. This transitio is not unusual for many materials.

We conclude from the differences in Figures 35 and 36 that recombination is apparently a significant controlling mechanism for permeation in this experiment.

4.0 CONCLUSIONS

In the course of the work performed here, the TMAP7 code has been demonstrated in a wide variety of applications. Many of these are contrived problems for which analytical solutions are available. Agreement between solutions calculated by TMAP7 and those generated in a Microsoft Excel™ spreadsheet is excellent. A second group of problems constitute replications of actual experiments, the results of which appear in published journals. By making use of accepted values of transport parameters and some fitting constant values, it has been shown that TMAP7 gives results in good agreement with actual measurements. These two groups of exercises constitute the verification and validation of the TMAP7 code.

The major challenge in assembling the computational models is finding the necessary parameters for the various property values needed in the code. A further challenge with TMAP7 is one faced by many such codes, numerical convergence. This is managed with various control parameters to adjust the damping in time iteration.

TMAP7 represents a significant step forward in modeling gas interaction with structures and in enclosures.

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APPENDIX A
SPECIES EQUILIBRATION MODEL

Suppose that two homonuclear diatomic molecular species, A_2 and B_2, are in a volume *V*, and at time $t = 0$, are allowed to contact a catalytic surface of area *S* that supports the reaction

$$\frac{1}{2}A_2 + \frac{1}{2}B_2 \leftrightarrow AB\,. \tag{A-1}$$

Assume further that the molecular species have the same mass and chemical properties such that there is no enthalpy change associated with this reaction and only configurational entropy is driving the reaction. Then

$$\Delta G_f = -T\Delta s_f = -RT\ln 2 \tag{A-2}$$

The equilibrium constant for reaction (A-1) is then

$$K_{eq} = \exp\left(-\frac{\Delta G_f}{RT}\right) = 2 \tag{A-3}$$

The law of mass action then requires that in equilibrium,

$$\frac{[AB]}{[A_2]^{\frac{1}{2}}[B_1]^{\frac{1}{2}}} = 2 \tag{A-4}$$

or equivalently

$$P_{AB} = 2P_{A_2}^{\frac{1}{2}}P_{B_2}^{\frac{1}{2}} \tag{A-5}$$

The *AB* molecules come from the dissociation of A_2 and B_2 molecules such that for starting pressures $P_{A_2}^0$ and $P_{B_2}^0$, it must also be true that at equilibrium

$$P_{AB} = 2\frac{P_{A_2}^0 P_{B_2}^0}{P_{A_2}^0 + P_{B_2}^0} \tag{A-6}$$

Three different approaches to the dynamics of the equilibration process will now be explored, one corresponding to *ratedep* boundary conditions, one to *surfdep* conditions, and finally one to *lawdep* diffusion boundary conditions.

Ratedep Conditions

At equilibrium, when Sieverts' law applies, for atom concentrations C_A and C_B at the surface,

$$\begin{aligned} C_A &= K_s\sqrt{P_{A_2}} \\ C_B &= K_s\sqrt{P_{B_2}} \end{aligned} \tag{A-7}$$

where K_s is the Sieverts' solubility.[a] Because we are considering isotopic variants, K_s will be the same for each homonuclear species. We expect also that under equilibrium conditions

$$K_d P_{A_2} = K_r C_A^2 \tag{A-8}$$

where K_d is the dissociation coefficient and K_r is the recombination coefficient. That leads to

$$K_d = K_s^2 K_r \tag{A-9}$$

We expect further for the heteronuclear species

$$K_d P_{AB} = K_{r_{AB}} C_A C_B \tag{A-10}$$

Under *ratedep* conditions, equilibrium is not assumed, but the relationships between the coefficients are maintained. In particular, the recombination and dissociation coefficients are assumed to be independent of the surface species concentrations and gas partial pressures, respectively. If the species molecular masses and solubilities are assumed equal, the dissociation coefficients for *AB*, A_2, and B_2 molecules should be identical except that because two different microscopic processes can produce *AB* (*A* jumping to find *B* and *B* jumping to find *A*) and only one (*A* finding *A*) can form A_2, and similarly for B_2, we expect $K_{r_{AB}}$ to be twice K_r for the homonuclear molecules.

The net current of *AB* molecules from surface area *S* to the volume *V* is the rate of change of those molecules in the enclosure.

$$\frac{dN_{AB}}{dt} = S\left(2K_r C_A C_B - K_d P_{AB}\right) \tag{A-11}$$

Here, N_{AB} is the number of molecules of species *AB* in the enclosure. At steady state, we see from Equations (A-6) and (A-11) that

$$C_A C_B = \frac{K_d}{2K_r} P_{AB} = \frac{K_d P_{A_2}^0 P_{B_2}^0}{K_r\left(P_{A_2}^0 + P_{B_2}^0\right)} \tag{A-12}$$

If diffusion is small, the almost constant numbers of *A* and *B* atoms in the gas imply that $C_A C_B$ should have an almost constant value given by Equation (A-12) regardless of the isotopic species composition. Then, Equation (A-11) becomes

$$\frac{dP_{AB}}{dt} = \frac{S K_d kT}{V}\left[2\frac{P_{A_2}^0 P_{B_2}^0}{\left(P_{A_2}^0 + P_{B_2}^0\right)} - P_{AB}\right] \tag{A-13}$$

Equation (A-13) is solved by

$$P_{AB} = 2\frac{P_{A_2}^0 P_{B_2}^0}{\left(P_{A_2}^0 + P_{B_2}^0\right)}\left[1 - exp\left(-\frac{SK_d kT}{V}t\right)\right] \tag{A-14}$$

---

[a] Note that solubility is frequently given in units of moles of diatomic gas per unit volume and square root of pressure.That value must be doubled to give the atom concentration referred to here.

Surfdep **Conditions**

When *surfdep* conditions apply, there are again no assumptions about equilibrium except in the steady state. Then, the surface concentration of molecules is directly proportional to the gas over-pressure and we define a deposition rate constant by.

$$\hat{K}_d = \frac{1}{\sqrt{2\pi MkT}} \exp\left(-\frac{E_x}{kT}\right) \tag{A-15}$$

where M is the mass of any of the species molecules, assuming all are equal, and E_x is the adsorption barrier energy. For release of the molecular species from the surface,

$$\hat{K}_r = \upsilon_o exp\left(\frac{E_c - E_x}{kT}\right) \tag{A-16}$$

Here, υ_o is the Debye frequency and E_c is the surface binding energy. At steady-state, the flux to the surface will be balanced by flux from the surface, and surface concentration will be related to the gas over-pressure by

$$C_{m_s} = P_m \frac{\hat{K}_d}{\hat{K}_r} = \frac{P_m}{\upsilon_o \sqrt{2\pi MkT}} exp\left(-\frac{E_c}{kT}\right) \tag{A-17}$$

The conversion of A_2 and B_2 molecules to AB molecules requires several steps. First, homonuclear molecules in the gas must get to the surface. Next, they must dissociate. Then the individual surface atoms must migrate to sites where they encounter their conjugates. Here we assume there is a probability of unity of their combination once they find each other, but it need not be so. Finally, the AB molecule must leave the surface and return to the gas. We write equations for species continuity at the surface.

$$C_{AB}\left(\hat{K}_r + \hat{K}_b\right) = P_{AB}\, \hat{K}_d + C_A C_B \left(2D_s\lambda\right) \tag{A-18}$$

$$C_{A_2}\left(\hat{K}_r + \hat{K}_b\right) = P_{A_2}\, \hat{K}_d + C_A^2 \left(D_s\lambda\right) \tag{A-19}$$

$$C_{B_2}\left(\hat{K}_r + \hat{K}_b\right) = P_{B_2}\, \hat{K}_d + C_B^2 \left(D_s\lambda\right) \tag{A-20}$$

$$C_A\left[\left(C_A + C_B\right)2D_s\lambda\right] = \left(C_{AB} + 2C_{A_2}\right)\hat{K}_b \tag{A-21}$$

$$C_B\left[\left(C_A + C_B\right)2D_s\lambda\right] = \left(C_{AB} + 2C_{B_2}\right)\hat{K}_b \tag{A-22}$$

In these equations, the dissociation rate for molecules at the surface is given by

$$\hat{K}_b = v_o\, exp\left(-\frac{E_b}{kT}\right) \tag{A-23}$$

Here, E_b is the dissociation activation energy, D_s is the surface diffusivity or mobility of the atomic species, and λ is the lattice constant, assumed to be the reciprocal cube root of the lattice density. For convenience $\hat{K}_b$ is assumed equal for all isotopic molecular species, though it need not be, and D_s is likewise assumed to be the same for all atomic species.

We may combine Equations (A-18) to (A-22) to find that

$$P_{total} = P_{A_2} + P_{B_2} + P_{AB} = \left(C_A + C_B\right)^2 \left(\frac{\hat{K}_r}{\hat{K}_b}\right) \frac{D\lambda}{\hat{K}_d} \tag{A-24}$$

This is reminiscent of Sieverts' law. With the conservation law for atoms in the gas assuming no diffusion or other losses

$$P_{AB} = 2\left(P^0_{A_2} - P_{A_2}\right) = 2\left(P^0_{B_2} - P_{B_2}\right) \tag{A-25}$$

Equation (A-24) becomes

$$\left(C_A + C_B\right)^2 = \left(P^0_{A_2} + P^0_{B_2}\right) \frac{\hat{K}_d}{D_s \lambda} \frac{\hat{K}_b}{\hat{K}_r} \tag{A-26}$$

It is supposed that the physical phenomena are always the same as they are in this situation.

The process that converts dissociation products to *AB* molecules is the recombination step while the net destruction rate is that for dissociation. Hence, similarly to Equation (A-11)

$$\frac{dN_{AB}}{dt} = S\left(C_A C_B \, 2D_s \lambda - C_{AB} \hat{K}_b\right) \tag{A-27}$$

Equation (A-18) must hold at all times such that if we solve it for C_{AB} and substitute the result into Equation (A-27) we get, successively

$$\begin{aligned}
\frac{dN_{AB}}{dt} &= S\left(C_A C_B \, 2D_s \lambda - \hat{K}_b \frac{P_{AB} \hat{K}_d + C_A C_B \, 2D_s \lambda}{\hat{K}_r + \hat{K}_b} \right) \\
\frac{dP_{AB}}{dt} &= \frac{SkT}{V} \left[C_A C_B \, 2D_s \lambda \left(1 - \frac{\hat{K}_b}{\hat{K}_r + \hat{K}_b} \right) - P_{AB} \frac{\hat{K}_d \hat{K}_b}{\hat{K}_r + \hat{K}_b} \right] \\
\frac{dP_{AB}}{dt} &= \frac{SkT}{V} \frac{\hat{K}_d \hat{K}_b}{\hat{K}_r + \hat{K}_b} \left[C_A C_B \, 2D\lambda \left(\frac{\hat{K}_r}{\hat{K}_d \hat{K}_b} \right) - P_{AB} \right]
\end{aligned} \tag{A-28}$$

This is solved by the expression

$$P_{AB} = C_A C_B \, 2D\lambda \, \frac{\hat{K}_r}{\hat{K}_d \hat{K}_b} \left[1 - exp\left(- \frac{SkT\, t}{V} \frac{\hat{K}_d \hat{K}_b}{\hat{K}_r + \hat{K}_b} \right) \right] \tag{A-29}$$

It may be shown, again using Equations (A-18) to (A-22), that this is equivalent to

$$P_{AB} = 2 \frac{P^0_{A_2} P^0_{B_2}}{P^0_{A_2} + P^0_{B_2}} \left[1 - \exp\left(-\frac{t}{\tau} \right) \right] \tag{A-30}$$

where

$$\tau = \frac{V\left(\hat{K}_r + \hat{K}_b\right)}{SkT \, \hat{K}_d \hat{K}_b} \tag{A-31}$$

This is identical with the time constant in Equation (A-14) for *ratedep* conditions if $\hat{K}_r << \hat{K}_b$.

Lawdep Conditions

Formally, when solution law boundary conditions are applied, it is not possible to have species conversion transients because the concentration at the surface is always fixed relative to the partial pressures in the gas over the surface, and there must, by definition, be a fixed gas mixture composition that will support the surface concentrations. Under *lawdep* diffusion boundary conditions, when heteronuclear species formation is involved, TMAP7 uses logic similar to that used in the *ratedep* and *surfdep* modes for the arrival rate of gas atoms to the surface. However, there are no barriers to adsorption or release, and conversion is assumed to take place instantaneously. Any gas that does not diffuse away is immediately reemitted from the surface. The simplistic solution is that gas arrives at the surface at a rate given by

$$J = P\hat{K}_d = \frac{P}{\sqrt{2\pi\, MkT}} \tag{A-32}$$

where P is the total pressure of the gas in the enclosure. The fraction of AB in that gas going to the surface is denoted by $\vec{\varphi}$. The gas leaving the surface is assumed to have its equilibrium mixture $\overleftarrow{\phi}$ where

$$\overleftarrow{\varphi} = \frac{2\sqrt{P_{A_2} P_{B_2}}}{P} \tag{A-33}$$

Then, as previously

$$\frac{d\,N_{AB}}{dt} = S\,J\left(\overleftarrow{\phi} - \vec{\phi}\right) \tag{A-34}$$

This becomes

$$\begin{aligned} \frac{d\,P_{AB}}{dt} &= \frac{SkT\,J}{V}\left(\frac{2\sqrt{P_{A_2} P_{B_2}} - P_{AB}}{P}\right) = \frac{SkT\,\hat{K}_d}{V}\left(2\sqrt{P_{A_2} P_{B_2}} - P_{AB}\right) \\ &= \frac{SkT\hat{K}_d}{V}\left(2\sqrt{P^o_{A_2} - \frac{P_{AB}}{2}}\sqrt{P^o_{B_2} - \frac{P_{AB}}{2}} - P_{AB}\right) \\ &= \frac{SkT\hat{K}_d}{V}\left(2\sqrt{P^o_{A_2} P^o_{B_2} - \left(P^o_{A_2} + P^o_{B_2}\right)\frac{P_{AB}}{2} + \frac{P^2_{AB}}{4}} - P_{AB}\right) \end{aligned} \tag{A-35}$$

This is a non-linear function, but consider that at early times, when P_{AB} is small, it is approximated by

$$\frac{d\,P_{AB}}{dt} \cong \frac{SkT\,\hat{K}_d}{V}\left(2\sqrt{P^o_{A_2} P^o_{B_2}} - P_{AB}\right) \tag{A-36}$$

whose solution is

$$P_{AB} = 2\sqrt{P^o_{A_2} P^o_{B_2}}\left[1 - \exp\left(-\frac{SkT\hat{K}_d}{V}t\right)\right] \tag{A-37}$$

If we consider the case of equal starting pressures of A_2 and B_2, then at the point where $P_{AB} = P_{A_2}$ $= P_{B_2}$

$$\frac{d\,P_{AB}}{dt} = \frac{SkT\hat{K}_d}{V} P_{AB} \tag{A-38}$$

At late times (approaching steady state)

$$P_{AB} = 2\sqrt{P_{A_2} P_{B_2}} \tag{A-39}$$

and the function is a constant.

APPENDIX B
TRAPPING PARAMETER DEVELOPMENT

The trapping parameter is a measure of the extent to which traps are filled under steady-state diffusion conditions. Consider a single trap of concentration ρ(x) in a material with lattice constant λ and trapping energy ε with a single diffusing species having mobile atom concentration *c*(x,t) with diffusivity *D* and trapped atom concentration c_t(x,t). The rate at which traps are filled is

$$\frac{\partial c_t(x,t)}{\partial t} = c(x,t)\frac{D}{\lambda^2}\left[\rho(x) - c_t(x,t)\right] - c_t(x,t)\nu_o \exp\left(-\frac{\varepsilon}{kT}\right) \tag{C-1}$$

At steady state, the net trapping rate is zero such that

$$c(x,t)\frac{D}{\lambda^2}\left[\rho(x) - c_t(x,t)\right] = c_t(x,t)\nu_o \exp\left(-\frac{\varepsilon}{kT}\right) \tag{C-2}$$

and

$$\frac{\rho(x)}{c_t(x,t)} = \frac{\lambda^2\,\nu_o}{c(x,t)D_o}\exp\left(\frac{E_d - \varepsilon}{kT}\right) + 1 \tag{C-3}$$

The trapped atom concentration can never exceed the trap concentration, but as the traps are fully filled, $\zeta \to 0$. When $\zeta >> 1$, the traps are nearly empty at steady state.

Now suppose (C-3) is recast as

$$\frac{c(x,t)}{c_t(x,t)} = \frac{\lambda^2\,\nu_o}{\rho\,D_o}\exp\left(\frac{E_d - \varepsilon}{kT}\right) + \frac{c(x,t)}{\rho} \equiv \zeta \tag{C-4}$$

and one considers the case where the first term in (C-4) dominates such that $\zeta >> \frac{c(x,t)}{\rho}$. This is called the *effective diffusivity* case because the ratio of mobile atom concentration to trapped atom concentration is independent of mobile atom concentration *c*(x,t). One then writes a modified diffusion equation as, successively,

$$\begin{aligned}
\frac{\partial c(x,t))}{\partial t} &= D\,\nabla^2 c(x,t)) - \frac{\partial c_t(x,t))}{\partial t} \\
&= D\,\nabla^2 c(x,t)) - \frac{c_t(x,t)}{c(x,t)}\frac{\partial c(x,t))}{\partial t} \\
&= D\,\nabla^2 c(x,t)) - \frac{1}{\zeta}\frac{\partial c(x,t))}{\partial t} \\
\frac{\partial c(x,t))}{\partial t}\left(1 + \frac{1}{\zeta}\right) &= D\,\nabla^2 c(x,t))
\end{aligned} \tag{C-5}$$

and finally

$$\frac{\partial c(x,t))}{\partial t} = \frac{D}{1+\frac{1}{\zeta}} \nabla^2 c(x,t)) \equiv D_{eff} \nabla^2 c(x,t)) \qquad \text{(C-6)}$$

whence the definition of effective diffusivity.

The opposite limit is the strong trapping case, in which $\zeta \approx \frac{c(x,t)}{\rho(x)}$ and essentially all the traps are filled. There, as gas atoms diffuse through the empty medium from an instantaneous application of a diffusing species concentration c_o at one edge of a slab, there is a trapping front at distance x from the front face beyond which the diffusing atoms cannot migrate until the local traps are filled. In equation form,

$$\rho(x)\,dx = \frac{c_o}{x} D\,dt \qquad \text{(C-7)}$$

Integration from time 0 to time τ when the front has progressed through the thickness L for uniform ρ results in an expression for the breakthrough time

$$\tau = \frac{L^2 \rho}{2D\,c_o} \qquad \text{(C-8)}$$

APPENDIX C
PROBLEM INPUT FILE LISTINGS

In this appendix are the input file listings used in the demonstration problems in Sections 2 and 3. These may be used as starting points for individual problems by the user.

Problem 1a: Diffusion from a Depleting Source (Val-1a)

```
title input
 Validation Problem #1  Tritium diffusion through SiC layer
 with depleting source at 2100C.  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,end
etemp=2373.0,end
esppres=ts,1.0e6,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,end
delx=0.0,3.0e-6,6*5e-6,0.,end
tempd=9*2373.0,end              $  Initial temperatures=(K)
$
end of thermal input
$
diffusion input
$
start diffseg,end
$ Sample [DIFFSEG 1]
nbrden=4.832e28,end
concd=t,9*0.0,end
qstrdr=t,equ,3,end              $ Q*/R for Soret effect unknown
dcoef=t,equ,1,end               $ Diffusion coeff (m2/s)
srcsd=t,equ,3,srcpf,9*0.0,end
difbcr=lawdep,encl,1,dspc,t,ts,pexp,1.0,solcon,equ,2,end
difbcl=sconc,dspc,t,conc,const,0.0,end
surfa=2.16e-6,end
$
end of diffusion input
$
equation input
$ (1) Diffusion coefficient
y=1.58e-4*exp(-308000.0/(8.314*temp)),end
$ (2) Solubility constant
```

```
y=7.244e22/temp,end
$ (3) Soret coefficient
y=0.0,end
end of equation input
$
table input
end of table input
$
control input
time=0.0,end                         $  initial time
tstep=0.1,end                        $  time step = 0.1 sec
timend=140.001,end                   $  the last time computed (s)
nprint=1000,end                      $  print every 10 seconds
itermx=2000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
plot input
nplot=10,end          $ makes plotfile entry every 1 sec
plotseg=1,end         $ segments for which plot info is needed
plotencl=1,2,end      $ enclosures for which plot info is needed
dname=t,end           $ diffusing species for which plot info is needed
ename=ts,end          $ enclosure species for which plot info is needed
dplot=sflux,moblinv,end
eplot=press,end       $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1b: Diffusion in a Semi-Infinite Slab with Constant-Source Boundary (Val-1b)

```
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=200,end
nbrencl=2,end
end of main input
$
enclosure input
start bdry,1,end
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,end
$delx=0.0,.001,.005,.01,.05,.1,.5,1.,5.,89*10.,0.0,end
delx = 0.0,198*0.1,0.0,end
tempd=200*2373.0,end
end of thermal input
$
diffusion input
start diffseg,end
nbrden=4.832e28,end
concd=t,200*0.0,end
qstrdr=t,equ,2,end
dcoef=t,const,1.0,end
srcsd=t,const,0.0,srcpf,200*0.0,end
difbcl=sconc,dspc,t,conc,const,1.0,end
difbcr=sconc,dspc,t,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=0.01,end                      $  time step = 10 msec
timend=50.0,end                     $  after implantation and desorption
nprint=500,end                      $  print every 10 seconds
```

```
itermx=20000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
plot input
nplot=100,end           $ makes plotfile entry every 1 sec
plotseg=1,end           $ segments for which plot info is needed
plotencl=1,2,end        $ enclosures for which plot info is needed
dname=t,end             $ diffusing species for which plot info is needed
ename=ts,end            $ enclosure species for which plot info is needed
dplot=sflux,end
eplot=end               $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1c Diffusion in a Partially Preloaded Semi-Infinite Slab (Val-1c)

```
title input
  Validation Problem #3 - Transient Concentration for semi-infinite,
  partially preloaded slab with both boundaries at 0 Concentration
  T = 2100 K
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=td,end
espcnme=t,end
segnds=99,end
nbrencl=2,end
end of main input
$
$ ---------------------------
enclosure input
$ ---------------------------
start bdry,1,end
etemp=2373.0,end
esppres=t,0.0,end
$
start bdry,2,end
etemp=2373.0,end
esppres=t,0.0,end
$
end of enclosure input
$
$ ----------------------------
thermal input
$ ----------------------------
start thermseg,end
delx=0.0,75*1.0,22*100.0,0.0,end
tempd=99*2373.0,end
$
end of thermal input
$ ---------------------------
diffusion input
$ ---------------------------
start diffseg,end
$ Sample [DIFFSEG 1]
nbrden=4.832e28,end
concd=td,11*1.0,88*0.0,end
qstrdr=td,equ,2,end     $ Q*/R for Soret effect unknown
dcoef=td,equ,1,end               $ Diffusion coeff (m2/s)
srcsd=td,equ,2,srcpf,99*0.0,end
difbcl=sconc,dspc,td,conc,const,0.0,end
difbcr=sconc,dspc,td,conc,const,0.0,end
surfa=1.0,end              $ 100 mm dia spot
end of diffusion input
$
$ ---------------------------
equation input
$ ---------------------------
$ (1)
```

```
y=1.0,end
$ (2)
y=0.0,end
$ (3)
end of equation input
$
$ ----------------------------
table input
$ ----------------------------
end of table input
$
$ ----------------------------
control input
$ ----------------------------
time=0.0,end
tstep=0.005,end         $  time step = 1 sec
timend=100.005,end     $  after implantation and desorption
nprint=1000,end         $  print every 40 seconds
itermx=20000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
$ ----------------------------
plot input
$ ----------------------------
nplot=1000,end         $ makes plotfile entry every 10 sec
plotseg=1,end         $ segments for which plot info is needed
plotencl=1,end        $ enclosures for which plot info is needed
dname=td,end          $ diffusing species for which plot info is needed
ename=t,end           $ enclosure species for which plot info is needed
dplot=moblinv,sflux,sconc,end
eplot=diff,end   $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1da. Effective Diffusivity Trap (Val-1da)

```
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,end
etemp=1000.0,end
esppres=t,1.0,end
$
start bdry,2,end
etemp=1000.0,end
esppres=t,0.0,end
end of enclosure input
$
thermal input
start thermseg,end
delx=0.0,20*0.05,0.0,end
tempd=22*1000.0,end
end of thermal input
$
diffusion input
start diffseg,end
$ Sample [DIFFSEG 1]
nbrden=3.1622e22,end
concd=td,22*0.0,end
qstrdr=td,const,0.0,end          $ Q*/R for Soret effect unknown
dcoef=td,equ,1,end               $ Diffusion coeff (m2/s)
srcsd=td,const,0.0,srcpf,22*0.0,end
trapping=ttyp,1,tconc,const,.1,tspc,td,alpht
         equ,2,alphr,equ,3,ctrap,const,0.0,end
difbcl=sconc,dspc,td,conc,const,3.1622e18,end
difbcr=sconc,dspc,td,conc,const,0.0,end
surfa=1.0,end
end of diffusion input
$
equation input
$ (1) Diffusion coefficient
y=1.0,end
$ (2) Trap rate (1/s)
y=1.0e15,end
$ (3) Trap release rate (1/s)
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                    $  time step = 0.01 sec
timend=3.0,end                    $  after implantation and desorption
nprint=6,end                      $  print every 0.06 seconds
itermx=2000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
plot input
nplot=1,end          $ makes plotfile entry every 0.01 sec
plotseg=1,end        $ segments for which plot info is needed
plotencl=end         $ enclosures for which plot info is needed
dname=td,end         $ diffusing species for which plot info is needed
ename=end            $ enclosure species for which plot info is needed
dplot=sflux,end
eplot=end            $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1db. Strong Trap (Val-1db)

```
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,end
etemp=1000.0,end
esppres=t,const,1.0,end
$
start bdry,2,end
etemp=1000.0,end
esppres=t,const,0.0,end
end of enclosure input
$
$ ----------------------------
thermal input
$ ----------------------------
start thermseg,end
delx=0.0,20*0.05,0.0,end
tempd=22*1000.0,end
end of thermal input
$
$ --------------------------
diffusion input
$ --------------------------
start diffseg,end
$ Sample [DIFFSEG 1]
nbrden=3.1622e22,end
concd=td,22*0.0,end
qstrdr=td,equ,2,end     $ Q*/R for Soret effect unknown
dcoef=td,equ,1,end               $ Diffusion coeff (m2/s)
srcsd=td,equ,2,srcpf,22*0.0,end
trapping=ttyp,1,tconc,const,.1,tspc,td,alpht
         equ,3,alphr,equ,4,ctrap,const,0.0,end
difbcl=sconc,dspc,td,conc,const,3.1622e18,end
difbcr=sconc,dspc,td,conc,const,0.0,end
surfa=1.0,end
end of diffusion input
$
$ --------------------------
equation input
$ --------------------------
$ (1)
```

```
y=1.0,end
$ (2)
y=0.0,end
$ (3)
y=1.0e15,end
$ (4)
y=1.0e13*exp(-15000./temp),end
end of equation input
$
$ --------------------------
table input
$ --------------------------
end of table input
$
$ --------------------------
control input
$ --------------------------
time=0.0,end
tstep=1.0,end
timend=800.0,end
nprint=1,end
itermx=2000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
damp=0.5
end of control input
$
$ --------------------------
plot input
$ --------------------------
nplot=10,end       $ makes plotfile entry every 10 sec
plotseg=1,end      $ segments for which plot info is needed
plotencl=end       $ enclosures for which plot info is needed
dname=td,end       $ diffusing species for which plot info is needed
ename=end          $ enclosure species for which plot info is needed
dplot=sflux,end
eplot=end          $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1dc. Multiple Trap (Val-1dc)

```
title input
  Validation Problem #4c  -  Trapping in a slab of constant upstream
  concentration  -  multiple traps.
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,end
etemp=1000.0,end
esppres=t,const,1.0,end
$
start bdry,2,end
etemp=1000.0,end
esppres=t,const,0.0,end
end of enclosure input
$
$ ----------------------------
thermal input
$ ----------------------------
start thermseg,end
delx=0.0,20*0.05,0.0,end
tempd=22*1000.0,end
end of thermal input
$
$ ---------------------------
diffusion input
$ ---------------------------
start diffseg,end
$ Sample [DIFFSEG 1]
nbrden=3.1622e22,end
concd=td,22*0.0,end
qstrdr=td,equ,2,end     $ Q*/R for Soret effect unknown
dcoef=td,equ,1,end               $ Diffusion coeff (m2/s)
srcsd=td,equ,2,srcpf,22*0.0,end
trapping=ttyp,1,tconc,const,.1,tspc,td,alpht
          equ,3,alphr,equ,4,ctrap,const,0.0
         ttyp,2,tconc,const,.15,tspc,td,alpht
          equ,3,alphr,equ,5,ctrap,const,0.0
         ttyp,3,tconc,const,.2,tspc,td,alpht
          equ,3,alphr,equ,6,ctrap,const,0.0,end
difbcl=sconc,dspc,td,conc,const,3.1622e18,end
difbcr=sconc,dspc,td,conc,const,0.0,end
surfa=1.0,end
end of diffusion input
$
```

```
$ ----------------------------
equation input
$ ----------------------------
$ (1)
y=1.0,end
$ (2)
y=0.0,end
$ (3)
y=1.0e15,end
$ (4)
y=1.0e13*exp(-100./temp),end
$ (5)
y=1.0e13*exp(-500./temp),end
$ (6)
y=1.0e13*exp(-800./temp),end
end of equation input
$
$ ----------------------------
table input
$ ----------------------------
end of table input
$
$ ----------------------------
control input
$ ----------------------------
time=0.0,end
tstep=0.0001,end
timend=50.0,end
nprint=50000,end                     $  print every 5 seconds
itermx=2000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
$ ----------------------------
plot input
$ ----------------------------
nplot=10000,end     $ makes plotfile entry every 1 sec
plotseg=1,end       $ segments for which plot info is needed
plotencl=end        $ no enclosure plot info is needed
dname=td,end        $ diffusing species for which plot info is needed
ename=end           $ no enclosure species plot info needed
dplot=sflux,end
eplot=end           $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1dd. Diffusion in a slab with no trapping (Val-1dd)

```
title input
  Validation Problem #4d  -  Diffusion in a slab of constant upstream
  concentration  -  no traps.
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,end
etemp=1000.0,end
esppres=t,1.0,end
$
start bdry,2,end
etemp=1000.0,end
esppres=t,0.0,end
end of enclosure input
$
$ ----------------------------
thermal input
$ ----------------------------
start thermseg,end
delx=0.0,20*0.05,0.0,end
tempd=22*1000.0,end
$
end of thermal input
$ ---------------------------
diffusion input
$ ---------------------------
start diffseg,end
$ Sample [DIFFSEG 1]
nbrden=3.1622e22,end
concd=td,22*0.0,end
qstrdr=td,equ,2,end     $ Q*/R for Soret effect unknown
dcoef=td,equ,1,end      $ Diffusion coeff (m2/s)
srcsd=td,equ,2,srcpf,22*0.0,end
difbcl=sconc,dspc,td,conc,const,3.1622e18,end
difbcr=sconc,dspc,td,conc,const,0.0,end
surfa=1.0,end
end of diffusion input
$
$ ---------------------------
equation input
$ ---------------------------
$ (1)
y=1.0,end
$ (2)
```

```
y=0.0,end
$ (3)
y=1.0e15,end
$ (4)
y=1.0e13*exp(-100./temp),end
end of equation input
$
$ ---------------------------
table input
$ ---------------------------
end of table input
$
$ ---------------------------
control input
$ ---------------------------
time=0.0,end
tstep=0.0001,end     $  time step = 1 sec
timend=3.0,end       $  after implantation and desorption
nprint=1000,end      $  print every 0.1 seconds
itermx=200,end
delcmx=1.0e-5,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
$ ---------------------------
plot input
$ ---------------------------
nplot=500,end       $ makes plotfile entry every 0.05 sec
plotseg=1,end       $ segments for which plot info is needed
plotencl=end        $ enclosures for which plot info is needed
dname=td,end        $ diffusing species for which plot info is needed
ename=end           $ enclosure species not needed
dplot=sflux,end
eplot=end           $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1e: Diffusion with Composite Material Layers (Val-1e)

```
title input
  Validation Problem #5  -  Tritium diffusion through PyC/SiC layer in NPR
  fuel particles at 2100 C with constant source and no trapping.
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,end
etemp=2373.0,end
esppres=t,1.e6,end
$
$ -----------------------
start bdry,2,end
$ -----------------------
etemp=2373.0,end
esppres,t,0.0,end
end of enclosure input
$
$ -----------------------
thermal input
$ -----------------------
start thermseg,end
delx=0.0,3.0e-6,6*5.0e-6,0.0,end
tempd=9*2373.0,end
$
start thermseg,end
delx=0.0,6*1.05e-5,3.0e-6,0.0,end
tempd=9*2373.0,end
end of thermal input
$
$ -----------------------
diffusion input
$ -----------------------
start diffseg,end
$ [DIFFSEG 1] PyC
nbrden=4.8319e28,end
concd=td,9*0.0,end
qstrdr=td,const,0.0,end          $ Q*/R for Soret effect unknown
dcoef=td,equ,1,end               $ Diffusion coeff (m2/s)
srcsd=td,const,0.0,srcpf,9*0.0,end
difbcl=sconc,dspc,td,conc,const,3.0537e25,end
difbcr=link,td,solcon,equ,3,end
surfa=2.16e-6,end
```

```
$
start diffseg,end
$ [DIFFSEG 2] SiC
concd=td,9*0.0,end
dcoef=td,equ,2,end
qstrdr=td,const,0.0,end
srcsd=td,const,0.0,srcpf,9*0.0,end
difbcr=sconc,dspc,td,conc,const,0.0,end
difbcl=link,td,solcon,equ,3,end
surfa=2.16e-6,end
end of diffusion input
$
$ -----------------------
equation input
$ -----------------------
$ (1) Diffusion coefficient PyC
y=1.274e-7,end
$ (2) Diffusion coefficient SiC
y=2.622e-11,end
$ (3) Solubility
y=1.0,end
end of equation input
$
$ -----------------------
table input
$ -----------------------
end of table input
$
$ -----------------------
control input
$ -----------------------
time=0.0,end
tstep=0.001,end
timend=100.0,end
nprint=1000,end       $  print every 1 second
itermx=2000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
omega=1.3,end
end of control input
$
$ -----------------------
plot input
$ -----------------------
nplot=1000,end       $ makes plotfile entry every 1 sec
plotseg=1,end        $ segments for which plot info is needed
plotencl=1,2,end     $ enclosures for which plot info is needed
dname=td,end         $ diffusing species for which plot info is needed
ename=t,end          $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=diff,end       $ flow of molecules into enclosure not needed
end of plot input
$
end of data
```

Problem 1fa: Heat Sink/Source Problem (Val-1fa)

```
title input
  Validation Problem #6a  -  Model Utilizes TMAP4 Thermal Capabilities
  Head Conduction in Slab with Internal Heat Generation
end of title input
$
main input
  dspcnme=qd,end
  espcnme=q,end
  segnds=18,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 imput
  start thermseg,end
  delx=0.0,16*0.10,0.0,end
  tempd=18*1000.0,end
  tcon=const,10.0,end
  rhocp=const,1.0,end
  hsrc=const,1.0e4,srcpf,0.0,16*1.0,0.0,end
  htrbcl=adiab,end
  htrbcr=stemp,const,300.0,end
end of thermal input
$
diffusion input
  start diffseg,end
  nbrden=1.0,end
  concd=qd,18*0.0,end
  dcoef=qd,const,0.1,end
  qstrdr=qd,const,0.0,end
  srcsd=qd,const,0.0,srcpf,18*0.0,end
  difbcl=nonflow,end
  difbcr=sconc,dspc,qd,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=0.001,end
  timend=50.1,end
  nprint=10000,end
  itermx=200,end
```

```
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=100,end
  plotseg=end
  plotencl=1,end
  dname=qd,end
  ename=q,end
  dplot=end
  eplot=etemp,end
end of plot input
$
end of data
```

Problem 1fa: Heat Sink/Source Problem (Val-1fap)

```
title input
  Validation Problem #6a  -  Model Utilizes TMAP4 Thermal Capabilities
  Head Conduction in Slab with Internal Heat Generation
end of title input
$
$ ---------------------
main input
$ ---------------------
  dspcnme=qd,end
  espcnme=q,end
  segnds=50,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 imput
$ ---------------------
  start thermseg,end
  delx=0.0,48*0.033333,0.0,end
  tempd=50*1000.0,end
  tcon=const,10.0,end
  rhocp=const,1.0,end
  hsrc=const,1.0e4,srcpf,0.0,48*1.0,0.0,end
  htrbcl=adiab,end
  htrbcr=stemp,const,300.0,end
end of thermal input
$
$ ---------------------
diffusion input
$ ---------------------
  start diffseg,end
  nbrden=1.0,end
  concd=qd,50*0.0,end
  dcoef=qd,const,0.1,end
  qstrdr=qd,const,0.0,end
  srcsd=qd,const,0.0,srcpf,50*0.0,end
  difbcl=nonflow,end
  difbcr=sconc,dspc,qd,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=0.001,end
  timend=50.1,end
  nprint=10000,end
  itermx=200,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
$ ---------------------
plot input
$ ---------------------
  nplot=1000,end
  plotseg=end
  plotencl=1,end
  dname=end
  ename=q,end
  dplot=end
  eplot=etemp,end
end of plot input
$
end of data
```

Problem 1fb: Thermal Diffusion Transient (Val-1fb)

```
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 imput
$ ----------------------
  start thermseg,end
  delx=0.0,1.25e-1,14*2.5e-1,1.25e-1,0.0,end
  tempd=18*300.0,end
  tcon=const,100.0,end
  rhocp=const,100.0,end
  hsrc=const,0.0,srcpf,18*0.0,end
  htrbcl=stemp,const,400.0,end
  htrbcr=stemp,const,300.0,end
end of thermal input
$
$ ----------------------
diffusion input
$ ----------------------
  start diffseg,end
  nbrden=1.0,end
  concd=td,18*0.0,end
  dcoef=td,const,1.0,end
  qstrdr=td,const,0.0,end
  srcsd=td,const,0.0,srcpf,18*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=5.0,end
  nprint=10,end
  itermx=2000,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
$ ---------------------
plot input
$ ---------------------
  nplot=10,end
  plotseg=1,end
  plotencl=1,end
  dname=td,end
  ename=t,end
  dplot=sconc,end
  eplot=end
end of plot input
$
end of data
```

Problem 1fc: Conduction in Composite Structure with Constant Surface Temperatures (Val-1fc)

```
title input
  Validation Problem #6c  -  Model Utilizes TMAP4 Thermal Capabilities
  Prediction of Composite Slab Temperature as a Function of Time
end of title input
$
$
main input
  dspcnme=td,end
  espcnme=t,end
  segnds=22,22,end
  nbrencl=2,end
  linksegs=1,2,end
end of main input
$
$
enclosure input
  start bdry,1
    etemp=600.0,end
    esppres=t,0.0,end
  start bdry,2
    etemp=600.0,end
    esppres=t,0.0,end
end of enclosure input
$
$
thermal imput
  start thermseg,end
    delx=0.0,20*2.0e-2,0.0,end
    tempd=22*0.0,end
    tcon=const,401.0,end
    rhocp=const,3.4392e6,end
    hsrc=const,0.0,srcpf,22*0.0,end
    htrbcl=stemp,const,600.0,end
    htrbcr=link,end
    hgap=const,1.e12,end
  start thermseg,end
    delx=0.0,20*2.0e-2,0.0,end
    tempd=22*0.0,end
    tcon=const,80.2,end
    rhocp=const,3.5179e6,end
    hsrc=const,0.0,srcpf,22*0.0,end
    htrbcl=link,end
    htrbcr=stemp,const,0.0,end
end of thermal input
$
$
diffusion input
  start diffseg,end
    nbrden=1.0,end
    concd=td,22*0.0,end
    dcoef=td,const,117.0e-6,end
    qstrdr=td,const,0.0,end
    srcsd=td,const,0.0,srcpf,22*0.0,end
```

```
    difbcl=sconc,dspc,td,conc,const,600.0,end
    difbcr=link,td,solcon,const,1.0,end
    surfa=1.0,end

  start diffseg,end
    nbrden=1.0,end
    concd=td,22*0.0,end
    dcoef=td,const,23.1e-6,end
    qstrdr=td,const,0.0,end
    srcsd=td,const,0.0,srcpf,22*0.0,end
    difbcr=sconc,dspc,td,conc,const,0.0,end
    difbcl=link,td,solcon,const,1.0,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=0.005,end
  timend=150.005,end
  nprint=1000,end
  itermx=2000,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=1,end
  plotseg=1,end
  plotencl=1,end
  dname=td,end
  ename=t,end
  dplot=sconc,end
  eplot=end
end of plot input
$
end of data
```

Problem 1fc: Conduction in Composite Structure with Constant Surface Temperatures at 10,000 sec (Val-1fcs)

```
title input
  Validation Problem #6c  -  Model Utilizes TMAP7 Thermal Capabilities
  Prediction of Composite Slab Temperature as a Function of Time
end of title input
$
$
main input
  dspcnme=td,end
  espcnme=t,end
  segnds=22,22,end
  nbrencl=,end
  linksegs=1,2,end
end of main input
$
$
thermal imput
  start thermseg,end
    delx=0.0,20*2.0e-2,0.0,end
    tempd=22*0.0,end
    tcon=const,401.0,end
    rhocp=const,3.4392e6,end
    hsrc=const,0.0,srcpf,22*0.0,end
    htrbcl=stemp,const,600.0,end
    htrbcr=link,end
    hgap=const,1.e12,end
  start thermseg,end
    delx=0.0,20*2.0e-2,0.0,end
    tempd=22*0.0,end
    tcon=const,80.2,end
    rhocp=const,3.5179e6,end
    hsrc=const,0.0,srcpf,22*0.0,end
    htrbcl=link,end
    htrbcr=stemp,const,0.0,end
end of thermal input
$
$
diffusion input
  start diffseg,end
    nbrden=1.0,end
    concd=td,22*0.0,end
    dcoef=td,const,117.0e-6,end
    qstrdr=td,const,0.0,end
    srcsd=td,const,0.0,srcpf,22*0.0,end
    difbcl=sconc,dspc,td,conc,const,600.0,end
    difbcr=link,td,solcon,const,1.0,end
    surfa=1.0,end
  start diffseg,end
    nbrden=1.0,end
    concd=td,22*0.0,end
    dcoef=td,const,23.1e-6,end
    qstrdr=td,const,0.0,end
    srcsd=td,const,0.0,srcpf,22*0.0,end
```

```
    difbcr=sconc,dspc,td,conc,const,0.0,end
    difbcl=link,td,solcon,const,1.0,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=10000.,end
  nprint=1000,end
  itermx=2000,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=1000,end
  plotseg=1,end
  plotencl=1,end
  dname=td,end
  dplot=sconc,end
  eplot=end
end of plot input
$
end of data
```

Problem 1fd: Convective Heating (Val-1fd)

```
title input
  Validation Problem #6d  -  Model Utilizes TMAP4 Thermal Capabilities
  Heat Conduction in Semi-Infinite Copper Slab with Convection
end of title input
$
$
main input
  dspcnme=qd,end
  espcnme=q,end
  segnds=90,end
  nbrencl=1,end
end of main input
$
$
enclosure input
  start bdry,1
  etemp=500.0,end
  esppres=q,0.0,end
end of enclosure input
$
$
thermal input
  start thermseg,end
  delx=0.0,16*0.10,72*5.0,0.0,end
  tempd=90*100.0,end
  tcon=const,401.0,end
  rhocp=const,3.439e6,end
  hsrc=const,0.0,srcpf,0.0,88*0.0,0.0,end
  htrbcl=convec,const,200.0,encl,1,end
  htrbcr=stemp,const,0.0,end
end of thermal input
$
$
diffusion input
  start diffseg,end
  nbrden=1.0,end
  concd=qd,90*0.0,end
  dcoef=qd,const,0.1,end
  qstrdr=qd,const,0.0,end
  srcsd=qd,const,0.0,srcpf,90*0.0,end
  difbcl=nonflow,end
  difbcr=sconc,dspc,qd,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=0.01,end
  timend=30.01,end
  nprint=100,end
  itermx=200,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=100,end
  plotseg=end
  plotencl=1,end
  dname=qd,end
  ename=q,end
  dplot=end
  eplot=etemp,end
end of plot input
$
end of data
```

Problem 1ga: Simple Forward Reactions (Val-1ga)

```
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 imput
  start thermseg,end
  delx=0.0,1.0,0.0,end
  tempd=3*300.0,end
end of thermal input
$
diffusion input
  start diffseg,end
  nbrden=1.0,end
  concd=q,3*0.0,end
  dcoef=q,const,1.0,end
  qstrdr=q,const,0.0,end
  srcsd=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*conce(1)*conce(2),end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=0.01,end
  timend=400.01,end
  nprint=1000,end
```

```
  itermx=200,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,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=etemp,end
end of plot input
$
end of data
```

Problem 1gb: Simple Forward Reactions (Val-1gb)

```
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 imput
  start thermseg,end
  delx=0.0,1.0,0.0,end
  tempd=3*300.0,end
end of thermal input
$
diffusion input
  start diffseg,end
  nbrden=1.0,end
  concd=q,3*0.0,end
  dcoef=q,const,1.0,end
  qstrdr=q,const,0.0,end
  srcsd=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*conce(1)*conce(2),end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=0.01,end
  timend=400.01,end
  nprint=1000,end
```

```
  itermx=200,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,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=etemp,end
end of plot input
$
end of data
```

Problem 1gc: Series Reactions (Val-1gc)

```
title input
  Validation Problem #7c  -  Chemical Reaction in Series Problem
   a -> b -> c
end of title input
$
main input
  dspcnme=q,end
  espcnme=a,b,c,end
  segnds=3,end
  nbrencl=3,end
end of main input
$
enclosure input
  start func,1
  etemp=300.0,end
  esppres=a,1.0e-6,b,0.0,c,0.0,end
  reaction=nequ,2
    ratequ,1
    nreact,1,a,1.0,nprod,1,b,1.0
    ratequ,2
    nreact,1,b,1.0,nprod,1,c,1.0,end
  evol=1.5e-1,end
$  outflow=nbrflwp,1,qflow,const,1.0,rencl,3,end
$
  start bdry,2
  etemp=300.0,end
  esppres=a,const,1.0e-6,b,const,0.0,c,const,0.0,end
$  outflow=nbrflwp,1,qflow,const,1.0,rencl,1,end
$
  start bdry,3
  etemp=300.0,end
  esppres=a,const,1.0e-6,b,const,1.0e-6,c,const,1.0e-6,end
end of enclosure input
$
thermal imput
  start thermseg,end
  delx=0.0,1.0,0.0,end
  tempd=3*300.0,end
end of thermal input
$
diffusion input
  start diffseg,end
  nbrden=1.0,end
  concd=q,3*0.0,end
  dcoef=q,const,1.0,end
  qstrdr=q,const,0.0,end
  srcsd=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
$ (1)
```

```
y=1.25e-2*conce(1),end
$ (2)
y=2.5e-3*conce(2),end
end of equation input
$
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=0.1,end
  timend=901.0,end
  nprint=20,end
  itermx=200,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=50,end
  plotseg=end
  plotencl=1,end
  dname=end
  ename=a,b,c,end
  dplot=end
  eplot=pres,end
end of plot input
$
end of data
```

Problem 1ha: Three Enclosure Problem (Val-1ha)

```
title input
  Validation Problem #8a  -  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=303.0,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=303.0,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,end
  delx=0.0,1.0,0.0,end
  tempd=3*303.0,end
end of thermal input
$
diffusion input
  start diffseg,end
    nbrden=1.0e21,end
    concd=t,3*0.0,end
    dcoef=t,const,1.0,end
    qstrdr=t,const,0.0,end
    srcsd=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=0.0001,end
  timend=40.001,end
  nprint=10000,end
  itermx=20,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=100,end
  plotseg=end
  plotencl=2,3,end
  dname=end
  ename=t2,end
  dplot=end
  eplot=conv,end
end of plot input
$
end of data
```

Problem 1hb: Equilibrating Enclosures (Val-1hb)

```
title input
  Validation Problem #8b  -  System Problem with Different Starting
          Concentrations
end of title input
$
main input
  dspcnme=t,end
  espcnme=t2,d2,end
  segnds=3,end
  nbrencl=2,end
end of main input
$
enclosure input
  start func,1
    etemp=303.0,end
    esppres=t2,1.0,d2,0.0,end
    reaction=nequ,0,end
    evol=1.0,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,2,end
  start func,2
    etemp=303.0,end
    reaction = nequ,0,end
    esppres=t2,0.0,d2,1.0,end
    evol=1.0,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,1,end
end of enclosure input
$
thermal input
  start thermseg,end
  delx=0.0,1.0,0.0,end
  tempd=3*303.0,end
end of thermal input
$
diffusion input
  start diffseg,end
    nbrden=1.0e21,end
    concd=t,3*0.0,end
    dcoef=t,const,1.0,end
    qstrdr=t,const,0.0,end
    srcsd=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=0.001,end
```

```
  timend=40.001,end
  nprint=1000,end
  itermx=20,end
  delcmx=1.0e-6,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=100,end
  plotseg=end
  plotencl=2,3,end
  dname=end
  ename=t2,end
  dplot=end
  eplot=conv,end
end of plot input
$
end of data
```

Problem 1ia: Species Equilibration on a Reactive Surface with Equal Starting Pressures (Val-1ia)

```
title input
Problem #9a. Chemical equilibration on polycrystalline tungsten surface
using conventional dissociation-recombination boundary condition.
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=h,d,end
espcnme=h2,d2,hd,end
segnds=12,end
nbrencl=1,end                 $  test chamber
end of main input
$
$ --------------------------
enclosure input
$ --------------------------
start func,1,end              $ Test chamber where sample is
$ Enclosure 1 is the test chamber with equal starting pressures
etemp=const,1000.0,end
esppres=h2,1.0e4,d2,1.0e4,hd,1.0e-10,end
evol=1.0,end                  $ Assumed value of 1.0 m3
end of enclosure input
$
thermal input
start thermseg,end
$ 1-mm foil [THERMSEG 1]
delx=0.0,10*1.0e-4,0.0,end
tempd=12*1000.,end                  $ Constant temperature (K)
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 1-mm foil [DIFFSEG 1]
nbrden=6.25e28,end
concd=h,const,1.0,d,const,1.0,end  $ Starting mobile concentrations
qstrdr=h,const,0.0,d,const,0.0,end $ Q*/R for Soret effect unknown
dcoef=h,equ,1,d,equ,1,end
srcsd=h,const,0.0,srcpf,const,1.0,d,const,0.0,srcpf,const,1.0,end
difbcl=ratedep,encl,1,
           spc,h,exch,h2,ksubd,equ,2,h,ksubr,5.88e-26
                 exch,hd,ksubd,equ,2,d,ksubr,1.18e-25
           spc,d,exch,hd,ksubd,equ,2,h,ksubr,1.18e-25
                 exch,d2,ksubd,equ,2,d,ksubr,5.88e-26,end
difbcr=nonflow,end
surfa=0.0025,end                 $ 50 x 50 mm square
end of diffusion input
$
equation input
$ (1) Diffusivity for h in tungsten (m2/s)
y=4.1e-7*exp(-0.39/8.625e-5/temp),end
$ (2) Dissociation coefficient at full efficiency
y=1.85802e24/sqrt(temp),end
```

```
end of equation input
$
table input
end of table input
$
control input
time=0.,end
tstep=0.001,end
timend=6.1,end
nprint=200,end
itermx=15000,end
delcmx=1.e-7,end
bump=1.e-2,end
bound=4.0,end
omega=0.2,end
damp=0.5,end
end of control input
$
plot input
nplot=200,end           $ makes plotfile entry every 0.2 sec
plotseg=1,end          $ segments for which plot info is needed
plotencl=1,end         $ enclosures for which plot info is needed
dname=h,d,end          $ diffusing species for which plot info is needed
ename=h2,d2,hd,end     $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1ib: Species Ratedep Equilibration on a Reactive Surface with Unequal Starting Pressures (Val-1ib)

```
title input
Problem #9b. Chemical equilibration on polycrystalline tungsten surface
using conventional dissociation-recombination boundary condition.
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=h,d,end
espcnme=h2,d2,hd,end
segnds=12,end
nbrencl=1,end                 $  test chamber
end of main input
$
$ --------------------------
enclosure input
$ --------------------------
start func,1,end              $ Test chamber where sample is
$ Enclosure 1 is the test chamber with equal starting pressures
etemp=const,1000.0,end
esppres=h2,1.0e4,d2,1.0e5,hd,1.0e-10,end
evol=1.0,end                  $ Assumed value of 1.0 m3
end of enclosure input
$
thermal input
start thermseg,end
$ 1-mm foil [THERMSEG 1]
delx=0.0,10*1.0e-4,0.0,end
tempd=12*1000.,end                  $ Constant temperature (K)
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 1-mm foil [DIFFSEG 1]

nbrden=6.25e28,end
concd=h,const,1.0,d,const,1.0,end  $ Starting mobile concentrations
qstrdr=h,const,0.0,d,const,0.0,end $ Q*/R for Soret effect unknown
dcoef=h,equ,1,d,equ,1,end
srcsd=h,const,0.0,srcpf,const,1.0,d,const,0.0,srcpf,const,1.0,end
difbcr=ratedep,encl,1,
           spc,h,exch,h2,ksubd,equ,2,h,ksubr,1.29e-16
                 exch,hd,ksubd,equ,2,d,ksubr,2.58e-16
           spc,d,exch,hd,ksubd,equ,2,h,ksubr,2.58e-16
                 exch,d2,ksubd,equ,2,d,ksubr,1.29e-16,end
difbcl=nonflow,end
surfa=0.0025,end                 $ 50 x 50 mm square
end of diffusion input
$
equation input
$ (1) Diffusivity for h in tungsten (m2/s)
y=4.1e-7*exp(-3.39/8.625e-5/temp),end $modified from 0.39 eV
$ (2) Dissociation coefficient at full efficiency
```

```
y=1.85802e24/sqrt(temp),end
end of equation input
$
table input
end of table input
$
control input
time=0.,end
tstep=0.01,end
timend=6.1,end
nprint=100,end
itermx=1500,end
delcmx=1.e-6,end
bump=1.e-2,end
bound=2.0,end
omega=0.05,end
damp=0.05,end
end of control input
$
plot input
nplot=20,end          $ makes plotfile entry every 0.2 sec
plotseg=1,end         $ segments for which plot info is needed
plotencl=1,end        $ enclosures for which plot info is needed
dname=h,d,end         $ diffusing species for which plot info is needed
ename=h2,d2,hd,end    $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1ic: Species Surfdep Equilibration on a Reactive Surface with Equal Starting Pressures (Val-1ic)

```
title input
Problem #9c. Chemical equilibration on polycrystalline tungsten surface,
Surfdep diffusion boundary condition with equal starting pressures.
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=h,d,end
espcnme=h2g,d2g,hdg,end
sspcnme=h2,d2,hd,end
segnds=7,end
nbrencl=1,end                 $  test chamber
end of main input
$
enclosure input
start func,1,end              $ Test chamber where sample is
$ Enclosure 1 is the test chamber with equal starting pressures
etemp=const,1000.0,end
esppres=h2g,1.0e4,d2g,1.0e4,hdg,1.e-10,end
evol=1.0,end                  $ Assumed value of 1.0 m3
end of enclosure input
$
thermal input
start thermseg,end
$ 1-mm foil [THERMSEG 1]
delx=0.0,5*2.0e-4,0.0,end
tempd=7*1000.,end                  $ Constant temperature (K)
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 1-mm foil [DIFFSEG 1]
nbrden=6.25e28,end
concd=h,const,0.0,d,const,0.0,end  $ Starting mobile concentrations
ssconc=h2,1.0,0.0,d2,1.0,0.0,hd,1.0,0.0,end
dcoef=h,equ,1,d,equ,1,h2,equ,2,d2,equ,2,hd,equ,2,end
difbcr=surfdep,encl,1
   spc,h,nu,8.4e12,ec,-0.01,es,1.04
       comb,h,prob,1.0
       comb,d,prob,1.0
   spc,d,nu,8.4e12,ec,-0.01,es,1.04
       comb,h,prob,1.0
       comb,d,prob,1.0
   spc,h2,nu,8.4e12,ec,-0.01
       exch,h2g,amu,2.0,ex,0.05
       diss,h,h,eb,0.0
       form,h,h,prob,1.0
   spc,d2,nu,8.4e12,ec,-0.01
       exch,d2g,amu,2.0,ex,0.05
       diss,d,d,eb,0.0
       form,d,d,prob,1.0
   spc,hd,nu,8.4e12,ec,-0.01
```

```
       exch,hdg,amu,2.0,ex,0.05
       diss,h,d,eb,0.0
       form,h,d,prob,1.0,end
difbcl=nonflow,end
surfa=0.0025,end                 $ 50 x 50 mm square
end of diffusion input
$
equation input
$ (1) Diffusivity for h,d in tungsten (m2/s)
y=5.3167e-7*exp(-4529/temp),end
$ (2) Diffusivity for h2, d2, hd on tungsten syrface (m2/s)
y=5.3167e-7*exp(-4529/temp),end
end of equation input
$
table input
end of table input
$
control input
time=0.,end
tstep=0.001,end
timend=10.,end
nprint=10,end
itermx=30000,end
delcmx=1.e-8,end
bump=1.e-4,end
bound=4.0,end
omega=0.9,end
damp=0.5,end
end of control input
$
plot input
nplot=200,end          $ makes plotfile entry every 0.2 sec
plotseg=1,end          $ segments for which plot info is needed
plotencl=1,end         $ enclosures for which plot info is needed
dname=h,d,end          $ diffusing species for which plot info is needed
sname=h2,d2,hd,end     $ surface species for which plot info is needed
ename=h2g,d2g,hdg,end $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1id: Species Surfdep Equilibration on a Reactive Surface with Unequal Starting Pressures (Val-1id)

```
title input
Problem #9d. Chemical equilibration on polycrystalline tungsten surface.
Surfdep boundaries with nequal starting pressures but 1.0-eV barrier energy.
end of title input
$ --------------------------
main input
$ --------------------------

dspcnme=h,d,end
espcnme=h2g,d2g,hdg,end
sspcnme=h2,d2,hd,end
segnds=7,end
nbrencl=1,end                 $  test chamber
end of main input
$
enclosure input
start func,1,end              $ Test chamber where sample is
$ Enclosure 1 is the test chamber with equal starting pressures
etemp=const,1000.0,end
esppres=h2g,1.0e4,d2g,1.0e4,hdg,1.e-10,end
evol=1.0,end                  $ Assumed value of 1.0 m3
end of enclosure input
$
thermal input
start thermseg,end
$ 1-mm foil [THERMSEG 1]
delx=0.0,5*2.0e-4,0.0,end
tempd=7*1000.,end                  $ Constant temperature (K)
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 1-mm foil [DIFFSEG 1]
nbrden=6.25e28,end
concd=h,const,0.0e00,d,const,0.0e0,end  $ Starting mobile concentrations
ssconc=h2,1.0,1.0,d2,1.0,1.0,hd,1.0,1.0,end
qstrdr=h,const,0.0,d,const,0.0,end $ Q*/R for Soret effect unknown
dcoef=h,equ,1,d,equ,1,h2,equ,1,d2,equ,1,hd,equ,1,end
srcsd=h,const,0.0,srcpf,const,1.0,d,const,0.0,srcpf,const,1.0,end
difbcl=surfdep,encl,1
   spc,h,nu,8.4e12,ec,-0.01,es,1.04
       comb,h,prob,1.0
       comb,d,prob,1.0
   spc,d,nu,8.4e12,ec,-0.01,es,1.04
       comb,h,prob,1.0
       comb,d,prob,1.0
   spc,h2,nu,8.4e12,ec,-0.01
       exch,h2g,amu,2.0,ex,0.2
       diss,h,h,eb,0.0
       form,h,h,prob,1.0
   spc,d2,nu,8.4e12,ec,-0.01
       exch,d2g,amu,2.0,ex,0.2
```

```
        diss,d,d,eb,0.0
        form,d,d,prob,1.0
    spc,hd,nu,8.4e12,ec,-0.01
        exch,hdg,amu,2.0,ex,0.2
        diss,h,d,eb,0.0
        form,h,d,prob,1.0,end
difbcr=nonflow,end
surfa=0.0025,end                 $ 50 x 50 mm square
end of diffusion input
$
equation input
$ (1) Diffusivity for h,d in tungsten (m2/s)
y=5.33e-7*exp(-0.39/8.625e-5/temp),end
end of equation input
$
table input
end of table input
$
control input
time=0.,end
tstep=0.001,end
timend=10.,end
nprint=100,end
itermx=90000,end
delcmx=1.e-7,end
bump=1.e-4,end
bound=4.0,end
omega=0.9,end
damp=0.2
end of control input
$
plot input
nplot=200,end         $ makes plotfile entry every 0.2 sec
plotseg=1,end         $ segments for which plot info is needed
plotencl=1,end        $ enclosures for which plot info is needed
dname=h,d,end         $ diffusing species for which plot info is needed
sname=h2,d2,hd,end    $ surface species for which plot info is needed
ename=h2g,d2g,hdg,end $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1ie: Species Lawdep Equilibration on a Reactive Surface with Equal Starting Pressures (Val-1ie)

```
title input
Problem #9e. Chemical equilibration on polycrystalline tungsten surface
using solution law dependent boundary condition.
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=h,d,end
espcnme=h2,d2,hd,end
segnds=12,end
nbrencl=1,end                 $  test chamber
end of main input
$
$ --------------------------
enclosure input
$ --------------------------
start func,1,end              $ Test chamber where sample is
$ Enclosure 1 is the test chamber with equal starting pressures
etemp=const,1000.0,end
esppres=h2,1.0e4,d2,1.0e4,hd,1.0e-10,end
espcomb=hd,amu,3,eta,const,2.0
   h2,amu,2.,pexp,0.5
   d2,amu,4.,pexp,0.5,end
evol=1.0,end                  $ Assumed value of 1.0 m3
end of enclosure input
$
thermal input
start thermseg,end
$ 1-mm foil [THERMSEG 1]
delx=0.0,10*1.0e-4,0.0,end
tempd=12*1000.,end                  $ Constant temperature (K)
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 1-mm foil [DIFFSEG 1]
nbrden=6.25e28,end
concd=h,const,1.0,d,const,1.0,end  $ Starting mobile concentrations
dcoef=h,equ,1,d,equ,1,end
difbcl=lawdep,encl,1,
           dspc,h,h2,pexp,0.5,solcon,equ,3
           dspc,d,d2,pexp,0.5,solcon,equ,3,end
difbcr=nonflow,end
surfa=0.0025,end                 $ 50 x 50 mm square
end of diffusion input
$
equation input
$ (1) Diffusivity for h in tungsten (m2/s)
y=4.1e-7*exp(-0.39/8.625e-5/temp),end
$ (2) Dissociation coefficient at full efficiency
y=1.85802e24/sqrt(temp),end
$ (3) Solubility for h in tungsten (atom/m3/Pa^.5)
```

```
y=1.e24,end
end of equation input
$
table input
end of table input
$
control input
time=0.,end
tstep=0.01,end
timend=6.1,end
nprint=100,end
itermx=1500,end
delcmx=1.e-6,end
bump=1.e-2,end
bound=2.0,end
omega=0.05,end
damp=0.05,end
end of control input
$
plot input
nplot=20,end          $ makes plotfile entry every 0.2 sec
plotseg=1,end         $ segments for which plot info is needed
plotencl=1,end        $ enclosures for which plot info is needed
dname=h,d,end         $ diffusing species for which plot info is needed
ename=h2,d2,hd,end    $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1if: Species Lawdep Equilibration on a Reactive Surface with Unequal Starting Pressures (Val-1if)

```
title input
Problem #9f. Chemical equilibration on polycrystalline tungsten surface
using solution law dependent boundary condition, unequal starting pressures.
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=h,d,end
espcnme=h2,d2,hd,end
segnds=12,end
nbrencl=1,end                  $  test chamber
end of main input
$
$ --------------------------
enclosure input
$ --------------------------
start func,1,end               $ Test chamber where sample is
$ Enclosure 1 is the test chamber with unequal starting pressures
etemp=const,1000.0,end
esppres=h2,1.0e4,d2,1.0e5,hd,1.0e-10,end
espcomb=hd,amu,3,eta,const,2.0
   h2,amu,2.,pexp,0.5
   d2,amu,4.,pexp,0.5,end
evol=1.0,end                   $ Assumed value of 1.0 m3
end of enclosure input
$
thermal input
start thermseg,end
$ 1-mm foil [THERMSEG 1]
delx=0.0,10*1.0e-4,0.0,end
tempd=12*1000.,end                   $ Constant temperature (K)
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 1-mm foil [DIFFSEG 1]
nbrden=6.25e28,end
concd=h,const,1.0,d,const,1.0,end  $ Starting mobile concentrations
dcoef=h,equ,1,d,equ,1,end
difbcl=lawdep,encl,1,
           dspc,h,h2,pexp,0.5,solcon,equ,3
           dspc,d,d2,pexp,0.5,solcon,equ,3,end
difbcr=nonflow,end
surfa=0.0025,end                  $ 50 x 50 mm square
end of diffusion input
$
equation input
$ (1) Diffusivity for h in tungsten (m2/s)
y=4.1e-7*exp(-0.39/8.625e-5/temp),end
$ (2) Dissociation coefficient at full efficiency
y=1.85802e24/sqrt(temp),end
$ (3) Solubility for h in tungsten (atom/m3/Pa^.5)
```

```
y=1.e24,end
end of equation input
$
table input
end of table input
$
control input
time=0.,end
tstep=0.01,end
timend=6.1,end
nprint=100,end
itermx=1500,end
delcmx=1.e-6,end
bump=1.e-2,end
bound=2.0,end
omega=0.05,end
damp=0.05,end
end of control input
$
plot input
nplot=20,end           $ makes plotfile entry every 0.2 sec
plotseg=1,end          $ segments for which plot info is needed
plotencl=1,end         $ enclosures for which plot info is needed
dname=h,d,end          $ diffusing species for which plot info is needed
ename=h2,d2,hd,end     $ enclosure species for which plot info is needed
dplot=moblinv,end
eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1ja: Radioactive Decay of Mobile Tritium in a Slab (Val-1ja)

```
title input
 Validation Problem #10a -   Simple decay in lattice
    T  -- >   He-3
end of title input
$
main input
dspcnme=t,he,end
dkrate=t,1.782411e-9,he,end
segnds=17,end
nbrencl=,end
end of main input
$
thermal input
start thermseg,end
delx=0.0,15*0.1,0.0,end
tempd=17*273.0,end
end of thermal input
$
diffusion input
start diffseg,end
nbrden=4.832e28,end
concd=t,17*1.0,he,17*0.0,end
qstrdr=t,const,0.0,he,const,0.0,end
dcoef=t,equ,1,he,const,0.0,end
srcsd=t,const,0.0,srcpf,17*0.0,he,const,0.0,srcpf,17*0.0,end
difbcl=nonflow,end
difbcr=nonflow,end
surfa=1.0,end
end of diffusion input
$
equation input
$ (1) Diffusivity for t
y=1.58e-4*exp(-308000.0/(8.314*temp)),end
$ (2) Trap release frequency
y=1.0e13*exp(-4.2/8.124e-5/temp),end
$ (3) Trapping frequency for t
y=2.096e15*exp(-308000.0/(8.314*temp)),end
end of equation input
$
table input
end of table input
$
control input
time=0.0,end
tstep=1.15e5,end                      $  time step = .01 year
timend=1.4197e9,end                   $  45 years
nprint=100,end                        $  print every year
itermx=20000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
damp=0.7,end
omega=1.3,end
end of control input
```

```
$
plot input
nplot=300,end              $ makes plotfile entry every 1/10 year
plotseg=1,end              $ segments for which plot info is needed
plotencl=end               $ enclosure info is not needed
dname=t,he,end             $ diffusing species for which plot info is needed
ename=end                  $ enclosure species for which plot info is needed
dplot=moblinv,trapinv,end
eplot=end
end of plot input
$
end of data
```

Problem 1jb: Decay of Tritium in a Distributed Trap (Val-1jb)

```
title input
 Validation Problem #10b -   1st order decay in traps
    T  -- >   He-3
end of title input
$
main input
dspcnme=t,he,end
dkrate=t,1.782411e-9,he,end
espcnme=ts,end
segnds=17,end
nbrencl=1,end
end of main input
$
enclosure input
start bdry,1,end
etemp=273.0,end
esppres=ts,1.0e5,end
end of enclosure input
$
thermal input
start thermseg,end
delx=0.0,15*0.1,0.0,end
tempd=17*273.0,end
end of thermal input
$
diffusion input
start diffseg,end
nbrden=4.832e28,end
concd=t,17*1.0,he,17*0.0,end
qstrdr=t,const,0.0,he,const,0.0,end
dcoef=t,equ,1,he,const,0.0,end
srcsd=t,const,0.0,srcpf,17*0.0,he,const,0.0,srcpf,17*0.0,end
difbcl=nonflow,end
difbcr=nonflow,end
trapping=ttyp,1,tconc,norm,0.001,0.75,0.5,0.0,tspc,t,alphr,equ,2
         alpht,equ,3,ctrap,const,0.5,end
surfa=1.0,end
end of diffusion input
$
equation input
$ (1) Diffusivity for t
y=1.58e-4*exp(-308000.0/(8.314*temp)),end
$ (2) Trap release frequency
y=1.0e13*exp(-4.2/8.124e-5/temp),end
$ (3) Trapping frequency for t
y=2.096e15*exp(-308000.0/(8.314*temp)),end
end of equation input
$
table input
end of table input
$
control input
time=0.0,end
tstep=1.15e5,end                      $  time step = .01 year
```

```
timend=1.4197e9,end                   $  45 years
nprint=100,end                        $  print every year
itermx=20000,end
delcmx=1.0e-7,end
bump=1.e-2,end
bound=2.0,end
damp=0.7,end
omega=1.3,end
end of control input
$
plot input
nplot=250,end             $ makes plotfile entry every 1/10 year
plotseg=1,end             $ segments for which plot info is needed
plotencl=end              $ enclosure info is not needed
dname=t,he,end            $ diffusing species for which plot info is needed
ename=end                 $ enclosure species for which plot info is needed
dplot=moblinv,trapinv,end
eplot=end
end of plot input
$
end of data
```

Problem 1ka: Simple Volumetric Source (Val-1ka)

```
title input
Problem 10a. Volumetric source rate in one enclosure with no exit pathways.
end of title input
$
main input
  dspcnme=h,t,end
  espcnme,h2,ht,t2,end
  segnds=22,end
  nbrencl=2,end
end of main input
$
enclosure input
start func,1,end
   etemp,const,500.0,end
   esppres=h2,1.0e5,ht,1.e-9,t2,1.0e-9,end
   srcse=t2,const,1.0e20,end
   evol=0.1,end
start func,2,end
   etemp,const,500.0,end
   esppres=h2,1.e-10,ht,1.e-10,t2,1.e-10,end
   evol=0.2,end
end of enclosure input
$
thermal input
$  Segment 1
start thermseg,end
    delx=0.0,20*1.25e-5,0.0,end
    tempd=22*500.0,end
end of thermal input
$
diffusion input
$  Segment 1
start diffseg,end
    nbrden=6.806e28,end
    concd=h,22*0.01,t,22*0.01,end
    dcoef=h,equ,1,t,equ,1,end
    difbcl=nonflow,end
    difbcr=nonflow,end
    surfa=1.0,end
end of diffusion input
$
equation input
$ (1) Diffusivity of H,T
y=4.31e-6*exp(-2818./temp),end
$ (2) Solubility of H,T
y=1.082e20,end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=10.,end
```

```
  timend=10000.0,end
  nprint=100,end
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-3,end
  damp=0.7,end
  bound=2.,end
  omega=0.2,end
end of control input
$
plot input
  nplot=10,end
  plotseg=1,end
  plotencl=1,2,end
  dname=h,t,end
  ename=h2,ht,t2,end
  dplot=moblinv,sflux,end
  eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1kb: Henry’s Law Boundaries with No Volumetric Source (Val-1kb)

```
title input
Problem 10b. H2 and T2 in one enclosure coupled by a membrane
with Henry's law diffusion boundaries to a second enclosure with no source.
end of title input
$
main input
  dspcnme=h,t,end
  espcnme,h2,ht,t2,end
  segnds=22,end
  nbrencl=2,end
end of main input
$
enclosure input
start func,1,end
   etemp,const,500.0,end
   esppres=h2,1.0e5,ht,1.e-9,t2,1.0e5,end
   evol=0.1,end
start func,2,end
   etemp,const,500.0,end
   esppres=h2,1.e-10,ht,1.e-10,t2,1.e-10,end
   evol=0.2,end
end of enclosure input
$
thermal input
$  Segment 1
start thermseg,end
    delx=0.0,20*1.25e-5,0.0,end
    tempd=22*500.0,end
end of thermal input
$
diffusion input
$  Segment 1
start diffseg,end
    nbrden=6.806e28,end
    concd=h,22*0.01,t,22*0.01,end
    dcoef=h,equ,1,t,equ,1,end
    difbcl=lawdep,encl,1
       dspc,h,h2,pexp,1.0,solcon,equ,2
       dspc,t,t2,pexp,1.0,solcon,equ,2,end
    difbcr=lawdep,encl,2
       dspc,h,h2,pexp,1.0,solcon,equ,2
       dspc,t,t2,pexp,1.0,solcon,equ,2,end
    surfa=1.0,end
end of diffusion input
$
equation input
$ (1) Diffusivity of H,T
y=4.31e-6*exp(-2818./temp),end
$ (2) Solubility of H,T
y=1.082e20,end
end of equation input
$
table input
end of table input
```

```
$
control input
  time=0.0,end
  tstep=1.,end
  timend=10000.0,end
  nprint=1000,end
  itermx=9000,end
  delcmx=1.0e-6,end
  bump=1.e-3,end
  damp=0.05,end
  bound=2.,end
  omega=0.2,end
end of control input
$
plot input
  nplot=100,end
  plotseg=1,end
  plotencl=1,2,end
  dname=h,t,end
  ename=h2,ht,t2,end
  dplot=moblinv,sflux,end
  eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1kc: Sieverts' Law Boundaries with No Volumetric Source (Val-1kc)

```
title input
Problem 10c. Volumetric source rate in one enclosure coupled by a membrane
with Sieverts law diffusion boundaries to a second enclosure with no source.
end of title input
$
main input
  dspcnme=h,t,end
  espcnme,h2,ht,t2,end
  segnds=22,end
  nbrencl=2,end
end of main input
$
enclosure input
start func,1,end
   etemp,const,500.0,end
   esppres=h2,1.0e5,ht,1.e-9,t2,1.0e5,end
   espcomb=ht,amu,4,eta,const,2.0
     h2,amu,2,pexp,0.5
     t2,amu,6,pexp,0.5,end
   evol=0.1,end
start func,2,end
   etemp,const,500.0,end
   esppres=h2,1.e-10,ht,1.e-10,t2,1.e-10,end
   espcomb=ht,amu,4,eta,const,2.0
     h2,amu,2,pexp,0.5
     t2,amu,6,pexp,0.5,end
   evol=0.2,end
end of enclosure input
$
thermal input
$  Segment 1
start thermseg,end
    delx=0.0,20*1.25e-5,0.0,end
    tempd=22*500.0,end
end of thermal input
$
diffusion input
$  Segment 1
start diffseg,end
    nbrden=6.806e28,end
    concd=h,22*0.01,t,22*0.01,end
    dcoef=h,equ,1,t,equ,1,end
    difbcl=lawdep,encl,1
       dspc,h,h2,pexp,0.5,solcon,equ,2
       dspc,t,t2,pexp,0.5,solcon,equ,2,end
    difbcr=lawdep,encl,2
       dspc,h,h2,pexp,0.5,solcon,equ,2
       dspc,t,t2,pexp,0.5,solcon,equ,2,end
    surfa=1.0,end
end of diffusion input
$
equation input
$ (1) Diffusivity of H,T
y=4.31e-6*exp(-2818./temp),end
```

```
$ (2) Solubility of H,T
y=1.082e20,end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=0.0001,end
  timend=10000.,end
  nprint=1000000,end
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-3,end
  damp=0.7,end
  bound=4.,end
  omega=0.2,end
end of control input
$
plot input
  nplot=1000000,end
  plotseg=1,end
  plotencl=1,2,end
  dname=h,t,end
  ename=h2,ht,t2,end
  dplot=moblinv,sflux,end
  eplot=press,diff,end
end of plot input
$
end of data
```

Problem 1kd: Sieverts' Law Boundaries with Volumetric Source (Val-1kd)

```
title input
Problem 10d. Volumetric source rate in one enclosure coupled by a membrane
with Sieverts law diffusion boundaries to a second enclosure with a tritiuim
source on the upstream side.
end of title input
$
main input
  dspcnme=h,t,end
  espcnme,h2,ht,t2,end
  segnds=22,end
  nbrencl=2,end
end of main input
$
enclosure input
start func,1,end
   etemp,const,500.0,end
   esppres=h2,1.0e5,ht,1.e-9,t2,1.0e5,end
   espcomb=ht,amu,4,eta,const,2.0
     h2,amu,2,pexp,0.5
     t2,amu,6,pexp,0.5,end
   srcse=t2,1.0e23,end
   evol=0.1,end
start func,2,end
   etemp,const,500.0,end
   esppres=h2,1.e-10,ht,1.e-10,t2,1.e-10,end
   espcomb=ht,amu,4,eta,const,2.0
     h2,amu,2,pexp,0.5
     t2,amu,6,pexp,0.5,end
   evol=0.2,end
end of enclosure input
$
thermal input
$  Segment 1
start thermseg,end
    delx=0.0,20*1.25e-5,0.0,end
    tempd=22*500.0,end
end of thermal input
$
diffusion input
$  Segment 1
start diffseg,end
    nbrden=6.806e28,end
    concd=h,22*0.01,t,22*0.01,end
    dcoef=h,equ,1,t,equ,1,end
    difbcl=lawdep,encl,1
       dspc,h,h2,pexp,0.5,solcon,equ,2
       dspc,t,t2,pexp,0.5,solcon,equ,2,end
    difbcr=lawdep,encl,2
       dspc,h,h2,pexp,0.5,solcon,equ,2
       dspc,t,t2,pexp,0.5,solcon,equ,2,end
    surfa=1.0,end
end of diffusion input
$
equation input
```

```
$ (1) Diffusivity of H,T
y=4.31e-6*exp(-2818./temp),end
$ (2) Solubility of H,T
y=1.082e20,end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=0.0001,end
  timend=10000.,end
  nprint=1000000,end
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-3,end
  damp=0.7,end
  bound=4.,end
  omega=0.2,end
end of control input
$
plot input
  nplot=1000000,end
  plotseg=1,end
  plotencl=1,2,end
  dname=h,t,end
  ename=h2,ht,t2,end
  dplot=moblinv,sflux,end
  eplot=press,diff,end
end of plot input
$
end of data
```

Problem 2a: Ion Implantation Experiment (Val-2a)

```
title input
  Sample Problem #1 - Plasma driven premeation 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
    etemp=703.,end
    esppres=d2,tabl,1,end
$
  start bdry,2,end
    etemp=703.0,end
    esppres=d2,const,2.e-6,end
end of enclosure input
$
$
thermal input
  start thermseg,end
  delx=0.0,1.e-9,5*4.0e-9,1.0e-8,1.0e-7,1.0e-6
       1.0e-5,9*5.4319e-5,0.0,end
  tempd=21*703.0,end
end of thermal input
$
$
diffusion input
  start diffseg,end
    nbrden=6.45e28,end
    concd=d,21*0.0,end
    dcoef=d,const,3.0e-10,end
    qstrdr=d,const,0.0,end
    srcsd=d,tabl,2,srcpf,3*0.0,0.15,0.7,0.15,15*0.0,end
    difbcl=ratedep,encl,1,spc,d
           exch,d2,ksubd,equ,1,d,ksubr,equ,2,end
    difbcr=ratedep,encl,2,spc,d
           exch,d2,ksubd,const,1.7918e15,d,ksubr
           const,2.0e-31,end
    surfa=1.0,end
end of diffusion input
$
$
equation input
$ (1) Dissociation constant (d_2/M^2.s.Pa^1/2)
y= 8.959e18*(1.0-0.999997*exp(-1.2e-4*time)),end
$ (2) Recombination constant (m^4/d_2.s)
y= 7.e-27*(1.0-0.999997*exp(-1.2e-4*time)),end
end of equation input
```

```
$
$
table input
$ (1)  Upstream enclosure pressure history
0.0,4.0e-5,5820.0,4.0e-5,5820.1,9.0e-6,9060.0,9.0e-6,9060.1,4.0e-5
12160.0,4.0e-5,12160.1,9.0e-6,14472.0,1.9e-6,14472.1,4.0e-5,17678.0
4.0e-5,17678.1,9.0e-6,1.0e10,9.0e-6,end
$  (2) Implantation Flux (d/m2.s)
0.0,4.9e19,5820.0,4.9e19,5820.1,0.0,9060.0,0.0,9060.1,4.9e19
12160.0,4.9e19,12160.1,0.0,14472.0,0.0,14472.1,4.9e19,17678.0
4.9e19,17678.1,0.0,1.0e10,0.0,end
end of table input
$
$
control input
  time=0.0,end
  tstep=20.0,end
  timend=19200.0,end
  nprint=60,end
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=3,end
  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
```

Problem 2b: Diffusion Experiment in Beryllium (Val-2ba, Val-2bb)

Charging Segment (Val-2ba)

```
title input
  Sample Problem #2 - 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
  nbrencl=1,end
  linksegs=1,2,end
end of main input
$
enclosure input
  start bdry,1,end
    etemp=773.,end
    esppres=d2,equ,6,end
end of enclosure input
$
thermal input
$  Segment 1   -  BeO film
  start thermseg,end
    delx=0.0,18*1.0e-9,0.0,end
    tempd=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
    htrbcr=link,end
    hgap=const,1.e6,end
$  Segment 2   -  Be metal   -  half thick
  start themseg,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
    tempd=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
$  Segment 1   -  BeO flim
  start diffseg,end
    nbrden=1.0e20,end
    concd=d,20*0.0,end
    dcoef=d,equ,2,end
    qstrdr=d,const,0.0,end
    srcsd=d,const,0.0,srcpf,20*0.0,end
    difbcl=lawdep,encl,1,dspc,d,d2
           pexp,0.5,solcon,equ,3,end
    difbcr=link,d,solcon,equ,3,end
```

```
    surfa=1.04e-4,end
$
$  Segment 2  -  Be foil  -  foil thickness
  start diffseg,end
    nbrden=1.0,end
    concd=d,17*0.0,end
    dcoef=d,equ,4,end
    qstrdr=d,const,0.0,end
    srcsd=d,const,0.0,srcpf,17*0.0,end
    difbcl=link,d,solcon,equ,5,end
    difbcr=nonflow,end
    surfa=1.04e-4
end of diffusion input
$
equation input
$ (1) Temperature History Equation
y= 773.-int(time/180000.)*(1-exp(-(time-180000.)/2700.))*475.,end
$ (2) - (5) Diffusion and Solubility Equations
$     (2) D of d in BeO (Fowler 1)
      y= 1.40e-4*exp(-24408./temp),end
$     (3) S for d in BeO
      y=5.00e20*exp(9377.7/temp),end
$     (4) D of D in Be (Abramov Be-2)
      y=8.0e-9*exp(-4220./temp),end
$     (5) S for d in Be  (Swansiger)
      y=7.156e27*exp(-11606./temp),end
$ (6)  Pressure History
y=13300.0*(1-int(time/180015.))+1.0e-6,end
end of equation input
$
$
table input
end of table input
$
$
control input
  time=0.0,end

  tstep=60.0,end
  timend=182400.0,end
  nprint=300,end
  itermx=90,end
  delcmx=1.0e-8,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=10,end
  plotseg=1,2,end
  plotencl=end
  dname=d,end
  ename=end
  dplot=moblinv,sflux,end
  eplot=end
end of plot input
```

```
$
end of data
```

Desorption Segment (Restart) (Val-2bb)

```
restart
$
equation input
$ (1) Temperature History Equation
y= 300.0+0.05*time,end
$ (2) - (5) Diffusion and Solubility Equations
$    (2) D of d in BeO (Fowler 1)
     y= 7.00e-5*exp(-27000./temp),end
$    (3) S for d in BeO
     y=5.00e20*exp(9377.7/temp),end
$    (4) D of D in Be (Abramov Be-2)
     y=8.0e-9*exp(-4220./temp),end
$    (5) S for d in Be  (Swansiger)
     y=7.156e27*exp(-11606./temp),end
$ (6)  Pressure History
y=0.001,end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=60.0,end
  timend=15460.0,end
  nprint=10,end
  itermx=90,end
  delcmx=1.0e-8,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=10,end
  plotseg=1,2,end
  plotencl=end
  dname=d,end
  ename=end
  dplot=moblinv,sflux,end
  eplot=end
end of plot input
$
end of data
```

Problem 2c: Test Cell Release Experiment (Val-2c)

```
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,1,end
    etemp=303.,end
    esppres=t2,0.434,ht,1.0e-30,hto,1.0e-30,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,2,end
    etemp=303.,end
    esppres=t2,const,0.,ht,const,0.,hto,const,0.
             h2o,const,714.,end
    outflow=nbrflwp,1,qflow,const,1.5e-5,rencl,1,end  $Low by 10*
  start bdry,3,end
    etemp=303.,end
    esppres=t2,const,0.0,ht,const,0.,hto,const,0.,h2o
             const,714.,end
end of enclosure input
$
thermal input
  start thermseg,end
    delx=0.0,10*1.6e-5,0.0,end
    tempd=12*303.0,end
end of thermal input
$
diffusion input
$  Segment 1
    start diffseg,end
    nbrden=1.0e20,end
    concd=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
    srcsd=t2d,const,0.0,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,1,dspc,t2d,t2,pexp,1.,solcon,const,4.e19
                         dspc,htd,ht,pexp,1.,solcon,const,4.e19
                         dspc,htod,hto,pexp,1.,solcon,const,6.e19
                         dspc,h2od,h2o,pexp,1.,solcon,const,6.e24,end
    difbcr=nonflow,end
    surfa=5.6,end
```

```
end of diffusion input
$
equation input
$ (1) - (2) Reaction Rate Equations
$ Index forc conc array is relative enclosure specie number
$     (i.e., t2=1, ht=2, hto=3, h2o=4)
$ (1)
y= 2.0e-29*conce(1)*(2.*conce(1)+conce(2)+conce(3)),end
$ (2)
y= 1.0e-29*conce(2)*(2.*conce(1)+conce(2)+conce(3)),end
end of equation input
$
table input
end of table input
$
control input
  time=0.0,end
  tstep=60.0,end
  timend=180000.0,end
  nprint=600,end
  itermx=90,end
  delcmx=1.0e-5,end
  bump=1.e-2,end
  bound=2.0,end
  omega=1.3,end
end of control input
$
plot input
  nplot=5,end
  plotseg=1,end
  plotencl=1,3,end
  dname=t2d,htd,htod,htod,end
  ename=t2,ht,hto,end
  dplot=moblinv,sflux,end
  eplot=pres,end
end of plot input
$
end of data
```

Problem 2d: Thermal Desorption Spectroscopy on Tungsten (Val-2d)

```
title input
Simulation of polycrystalline tungsten experiment irradiated at RT with
H at 5 keV, 1E15 H/cm2/s for 5000 s.  Then TDS at 50 C/min to 1000 C.
See T. Hino et al., Fus. Engr. & Des. 39-40 (1998) pp.227-233.
end of title input
$ --------------------------
main input
$ --------------------------
dspcnme=h,end
sspcnme=h2,end
espcnme=h2g,end
segnds=12,18,end              $ 1 implant zone 15 nm, 2 bulk 0.1 mm
nbrencl=3,end                 $ 1 test chamber, 2 source, 3 sink
linksegs=1,2,end
end of main input
$ ---------------------------
enclosure input
$ ---------------------------
start func,1,end              $ Test chamber where sample is
$ Enclosure 1 is the plasma chamber with pressure assumed negligible
etemp=tabl,1,end
esppres=h2g,1.0e-7,end
evol=0.1,end                  $ Assumed value of 0.1 m3
outflow=nbrflwp,1,qflow,const,0.0517,rencl,2,end
$
start bdry,2,end
$ Enclosure 2 is the sink for the vacuum pumping system
etemp=const,300.,end
esppres=h2g,const,1.e-8,end
$
start bdry,3,end
$ Enclosure 3 is the source for the test chamber (ion source)
etemp=const,300.,end
esppres=h2g,const,1.e-5,end
outflow=nbrflwp,1,qflow,const,0.0517,rencl,1,end
end of enclosure input
$ ----------------------------
thermal input
$ ----------------------------
start thermseg,end
$ 15-nm implantation zone [THERMSEG 1]
delx=0.0,10*1.5e-9,0.0,end
tempd=12*300.,end              $  Initial temperatures=(K)
tcon=equ,1,end                 $  W thermal cond. (W/m-K)
rhocp=equ,2,end                $  rho*cp for W  (J/m3K)
hsrc=const,0.,srcpf,12*0.,end  $  Neglect internal heat sources
htrbcl=stemp,tabl,1,end        $  Temperature at the plasma-side surface
htrbcr=link,end
hgap=const,1.e9,end            $  Effectively infinite gap conductance
$
start thermseg,end
$ Balance of 0.1-mm tungsten specimen [THERMSEG 2]
delx=0.,1.e-9,1.e-8,1.0e-7,1.0e-6,12*7.407e-6,0.0,end
tempd=18*300.,end              $  Initial temperatures=(K)
```

```
tcon=equ,1,end                 $  W thermal cond. (W/m-K)
rhocp=equ,2,end                $  rho*cp for W  (J/m3K)
hsrc=const,0.,srcpf,18*0.,end  $  Neglect internal heat sources
htrbcl=link,end                $  Temperature at the plasma-side surface
htrbcr=stemp,tabl,1,end        $  Temperature at the back-side surface
$
end of thermal input
$ ======================
diffusion input
$ ======================
start diffseg,end
$ 15-nm implantation zone [DIFFSEG 1]
nbrden=6.25e28,end
concd=h,const,1.0e-10,end       $ Starting mobile concentration
ssconc=h2,1.0,link,end          $ Starting surface species concentration
trapping=ttyp,1,tconc,norm,0.086,4.6e-9,1.0e-8,0.0,tspc,h,alphr,equ,4
             alpht,equ,3,ctrap,const,0.0
         ttyp,2,tconc,const,4.1e-3,tspc,h,alphr,equ,5
              alpht,equ,3,ctrap,const,4.4e-10
         ttyp,3,tconc,const,2.e-3,tspc,h,alphr,equ,6
              alpht,equ,3,ctrap,const,1.4e-10,end
qstrdr=h,const,0.,end           $ Q*/R for Soret effect unknown
dcoef=h,equ,7,h2,equ,10,end     $ Diffusion coeff (m2/s) [Modified]
srcsd=h,tabl,2,srcpf,norm,1.0,4.6e-9,3.0e-9,0.0,end
difbcl=surfdep,encl,1
   spc,h,nu,8.4e12,ec,0.8,es,1.04
       comb,h,prob,1.0
   spc,h2,nu,8.4e12,ec,0.01
       exch,h2g,amu,2.0,ex,0.05
       diss,h,h,eb,1.42
       form,h,h,prob,1.0,end
difbcr=link,h,solcon,equ,8,end
surfa=0.0025,end                 $ 50 x 50 mm square
$
start diffseg,end
$ Balance of 0.1-mm tungsten specimen [DIFFSEG 2]
nbrden=6.25e28,end
concd=h,const,1.0e-10,end            $ Starting mobile concentration
ssconc=h2,link,1.0,end          $ Starting surface species concentration
trapping=ttyp,1,tconc,const,0.0,tspc,h,alphr,equ,4
             alpht,equ,3,ctrap,const,0.0
         ttyp,2,tconc,const,4.1e-3,tspc,h,alphr,equ,5
              alpht,equ,3,ctrap,const,4.4e-10
         ttyp,3,tconc,const,2.e-3,tspc,h,alphr,equ,6
              alpht,equ,3,ctrap,const,1.4e-10,end
qstrdr=h,const,0.,end           $ Q*/R for Soret effect unknown
dcoef=h,equ,9,h2,equ,10,end     $ Diffusion coeff (m2/s) [Modified]
srcsd=h,const,0.0,srcpf,18*0.0,end
difbcr=surfdep,encl,1
   spc,h,nu,8.4e12,ec,0.8,es,1.04
       comb,h,prob,1.0
   spc,h2,nu,8.4e12,ec,0.01
       exch,h2g,amu,2.0,ex,0.05
       diss,h,h,eb,1.42
       form,h,h,prob,1.0,end
difbcl=link,h,solcon,equ,8,end
surfa=0.0025,end                 $ 50 x 50 mm square
```

```
$
end of diffusion input
$
equation input
$ (1) Thermal conductivity of tungsten (W/m-K)
y=163.-0.0739*temp+2.89e-5*temp**2-4.3e-9*temp**3,end
$ (2) Rho Cp for tungsten (J/m3K)
y=(1930.-.0388*temp)*(131.+.0226*temp-5.73e-6*temp**2+3.69e-9
  *temp**3),end
$ (3) Alpht for h in tungsten (1/s)
y=9.1316e12*exp(-0.39/8.625e-5/temp),end
$ (4) Alphr for trap 1 in tungsten (1/s)
y=8.4e12*exp(-1.2/8.625e-5/temp),end
$ (5) Alphr for trap 2 in tungsten (1/s)
y=8.4e12*exp(-1.6/8.625e-5/temp),end
$ (6) Alphr for trap 3 in tungsten (1/s)
y=8.4e12*exp(-2.9/8.625e-5/temp),end
$ (7) Diffusivity for h in tungsten (m2/s)
y=4.1e-7*exp(-0.39/8.625e-5/temp),end
$ (8) Hydrogen solubility in tungsten (1/m3-Pa^1/2)
y=1.778e24*exp(-1.04/8.625e-5/temp),end
$ (9) Diffussivity for h in implant-layer tungsten (m2/s)[Modified]
y=4.1e-7*exp(-.39/8.625e-5/temp)*10.,end
$ (10) Surface diffusivity for h2 at tungsten surface (m2/s)
y=4.1e-7*exp(-.1/8.625e-5/temp),end
end of equation input
$
table input
$ (1) Temperature history of enclosure 1
0.,300.,5000.,300.,6200.,1273.,8000.,1273.,end
$ (2) Implantation flux history (atom/m2/s)
0.,1.e19,4800.,1.e19,4801.,0.0,1.e10,0.0,end
end of table input
$
control input
time=0.,end
tstep=.1,end
timend=6800.0,end                     $  after implantation and desorption
nprint=600,end                       $  print every 10  minutes
itermx=800000,end
delcmx=1.e-5,end
bump=1.e-2,end
bound=2.0,end
omega=0.9,end
damp=0.5,end
end of control input
$
plot input
nplot=300,end           $ makes plotfile entry every 30 sec
plotseg=1,2,end         $ segments for which plot info is needed
plotencl=1,end          $ enclosures for which plot info is needed
dname=h,end             $ diffusing species for which plot info is needed
ename=h2g,end           $ enclosure species for which plot info is needed
dplot=moblinv,trapinv,sflux,stemp,end
eplot=press,diff,end    $ flow of molecules into enclosure not needed
end of plot input
$
```

```
end of data
```

Problem 2ea: Permeation of D_2 through 0.05-mm Pd at 825 K (Val-2ea)

```
title input
  Sample Problem #5a - Co-Permeation of D and H through Pd by K. Kizu,
  A. Pisarev and T. Tanabe, Journal of Nuclear Materials, 289 (2001) 291-302.
  Pd 0.05 mm, 825 K, D2 only
end of title input
$
main input
  dspcnme=d,end
  espcnme=d2,end
  segnds=12,end
  nbrencl=5,end
end of main input
$
enclosure input
$
start bdry,1,end
$ This is the background pressure source for both active chambers
    etemp=tabl,1,end
    esppres d2,1.0e-6,end
    outflow=nbrflwp,2,qflow,const,0.1,rencl,2
                      qflow,const,0.1,rencl,3,end
$
start func,2,end
$ This is the upstream chamber connecting to the membrane
    etemp=tabl,1,end
    esppres=d2,1.e-6,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
$
start func,3,end
$ This is the downstream chamber connected to the membrane
    etemp=tabl,1,end
    esppres=d2,1.e-6,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
$
start bdry,4,end
$ This is the gas sink representing the vacuum pumping system
    etemp=tabl,1,end
    esppres d2,1.e-10,end
$
start bdry,5,end
$ This is the gas source with pre-programmed species pressures
    etemp=tabl,1,end
    esppres=d2,tabl,2,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,2,end
end of enclosure input
$
thermal input
$  Segment 1  -  Pd film
start thermseg,end
    delx=0.0,10*5.0e-6,0.0,end
    tempd=12*300.0,end
    tcon=const,73.,end
```

```
    rhocp=const,2.932e6,end
    hsrc=const,0.0,srcpf,12*0.0,end
    htrbcl=stemp,tabl,1,end
    htrbcr=stemp,tabl,1,end
end of thermal input
$
$
diffusion input
$  Segment 1  -  Pd flim
start diffseg,end
    nbrden=6.806e28,end
    concd=d,12*1.0e5,end
    dcoef=d,equ,2,end
    qstrdr=d,const,0.0,end
    srcsd=d,const,0.0,srcpf,12*0.0,end
    difbcr=lawdep,encl,2
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    difbcl=lawdep,encl,3
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    surfa=1.8e-4,end
end of diffusion input
$
$
equation input
$
$ (1) Diffusivity of H in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960)]
y=3.728e-4*exp(-1315.8/temp),end
$
$ (2) Diffusivity of D in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960); divided by 1.414 for isotope effect]
y=2.636e-4*exp(-1315.8/temp),end
$
$ (3) Solubility of H,D in Pd
$ From measurements of Kizu et al.
y=1.511e23*exp(-5918./temp),end
$
end of equation input
$
$
table input
$ (1) Temperature history
0.0,825.,8.e5,825.,end
$ (2) Pressure history of D2 in Enclosure 5
0.0,1.20e-04,150.,1.20e-4,151.,2.41e-4,250.,2.41e-4,251.,6.06e-4,350.,6.06e-4
351.,1.30e-3,450.,1.30e-3,451.,2.53e-3,550.,2.53e-3,551.,7.08e-3,650.
7.08e-3,651.,1.45e-2,750.,1.45e-2,751.,2.63e-2,850.,2.63e-2,851.,6.51e-2
950.,6.51e-2,951.,0.116,1050.,0.116,1051.,0.297,1150.,0.297,1151.,0.76,
1250.,0.76,1251.,1.55,1350.,1.55,1351.,3.37,1900.,3.37,end
end of table input
$
$
control input
  time=0.0,end
  tstep=0.1,end
  timend=1450.0,end
  nprint=500,end
```

```
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-3,end
  damp=0.7
  bound=4.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=1000,end
  plotseg=1,end
  plotencl=2,3,5,end
  dname=d,end
  ename=d2,end
  dplot=moblinv,sflux,end
  eplot=press,conv,diff,end
end of plot input
$
end of data
```

Problem 2eb: Permeation of D_2 through 0.025-mm Pd at 825 K (Val-2eb)

```
title input
  Sample Problem #5b - Co-Permeation of D and H through Pd by K. Kizu,
  A. Pisarev and T. Tanabe, Journal of Nuclear Materials, 289 (2001) 291-302.
  Pd 0.025 mm, 825 K, D2 only
end of title input
$
main input
  dspcnme=d,end
  espcnme=d2,end
  segnds=12,end
  nbrencl=5,end
end of main input
$
enclosure input
$
start bdry,1,end
$ This is the background pressure source for both active chambers
    etemp=tabl,1,end
    esppres d2,1.0e-6,end
    outflow=nbrflwp,2,qflow,const,0.1,rencl,2
                      qflow,const,0.1,rencl,3,end
$
start func,2,end
$ This is the upstream chamber connecting to the membrane
    etemp=tabl,1,end
    esppres=d2,1.e-6,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
$
start func,3,end
$ This is the downstream chamber connected to the membrane
    etemp=tabl,1,end
    esppres=d2,1.e-6,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
$
start bdry,4,end
$ This is the gas sink representing the vacuum pumping system
    etemp=tabl,1,end
    esppres d2,1.e-10,end
$
start bdry,5,end
$ This is the gas source with pre-programmed species pressures
    etemp=tabl,1,end
    esppres=d2,tabl,2,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,2,end
end of enclosure input
$
thermal input
$  Segment 1  -  Pd film
start thermseg,end
    delx=0.0,10*2.5e-6,0.0,end
    tempd=12*300.0,end
    tcon=const,73.,end
```

```
    rhocp=const,2.932e6,end
    hsrc=const,0.0,srcpf,12*0.0,end
    htrbcl=stemp,tabl,1,end
    htrbcr=stemp,tabl,1,end
end of thermal input
$
$
diffusion input
$  Segment 1  -  Pd flim
start diffseg,end
    nbrden=6.806e28,end
    concd=d,12*1.0e5,end
    dcoef=d,equ,2,end
    qstrdr=d,const,0.0,end
    srcsd=d,const,0.0,srcpf,12*0.0,end
    difbcr=lawdep,encl,2
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    difbcl=lawdep,encl,3
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    surfa=1.8e-4,end
end of diffusion input
$
$
equation input
$
$ (1) Diffusivity of H in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960)]
y=3.728e-4*exp(-1315.8/temp),end
$
$ (2) Diffusivity of D in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960); divided by 1.414 for isotope effect]
y=2.636e-4*exp(-1315.8/temp),end
$
$ (3) Solubility of H,D in Pd
$ From measurements of Kizu et al.
y=1.511e23*exp(-5918./temp),end
$
end of equation input
$
$
table input
$ (1) Temperature history
0.0,825.,8.e5,825.,end
$ (2) Pressure history of D2 in Enclosure 5
0.0,1.20e-04,150.,1.20e-4,151.,2.41e-4,250.,2.41e-4,251.,6.06e-4,350.,6.06e-4
351.,1.30e-3,450.,1.30e-3,451.,2.53e-3,550.,2.53e-3,551.,7.08e-3,650.
7.08e-3,651.,1.45e-2,750.,1.45e-2,751.,2.63e-2,850.,2.63e-2,851.,6.51e-2
950.,6.51e-2,951.,0.116,1050.,0.116,1051.,0.297,1150.,0.297,1151.,0.76,
1250.,0.76,1251.,1.55,1350.,1.55,1351.,3.37,1900.,3.37,end
end of table input
$
$
control input
  time=0.0,end
  tstep=0.1,end
  timend=1450.0,end
  nprint=500,end
```

```
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-3,end
  damp=0.7
  bound=4.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=1000,end
  plotseg=1,end
  plotencl=2,3,5,end
  dname=d,end
  ename=d2,end
  dplot=moblinv,sflux,end
  eplot=press,conv,diff,end
end of plot input
$
end of data
```

Problem 2ec: Permeation of D_2 through 0.025-mm Pd at 865 K (Val-2ec)

```
title input
  Sample Problem #5c - Co-Permeation of D and H through Pd by K. Kizu,
  A. Pisarev and T. Tanabe, Journal of Nuclear Materials, 289 (2001) 291-302.
  Pd 0.025 mm, 865 K, D2 only
end of title input
$
main input
  dspcnme=d,end
  espcnme=d2,end
  segnds=12,end
  nbrencl=5,end
end of main input
$
enclosure input
$
start bdry,1,end
$ This is the background pressure source for both active chambers
    etemp=tabl,1,end
    esppres d2,1.0e-6,end
    outflow=nbrflwp,2,qflow,const,0.1,rencl,2
                      qflow,const,0.1,rencl,3,end
$
start func,2,end
$ This is the upstream chamber connecting to the membrane
    etemp=tabl,1,end
    esppres=d2,1.e-6,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
$
start func,3,end
$ This is the downstream chamber connected to the membrane
    etemp=tabl,1,end
    esppres=d2,1.e-6,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
$
start bdry,4,end
$ This is the gas sink representing the vacuum pumping system
    etemp=tabl,1,end
    esppres d2,1.e-10,end
$
start bdry,5,end
$ This is the gas source with pre-programmed species pressures
    etemp=tabl,1,end
    esppres=d2,tabl,2,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,2,end
end of enclosure input
$
thermal input
$  Segment 1  -  Pd film
start thermseg,end
    delx=0.0,10*2.5e-6,0.0,end
    tempd=12*300.0,end
    tcon=const,73.,end
```

```
    rhocp=const,2.932e6,end
    hsrc=const,0.0,srcpf,12*0.0,end
    htrbcl=stemp,tabl,1,end
    htrbcr=stemp,tabl,1,end
end of thermal input
$
$
diffusion input
$  Segment 1  -  Pd flim
start diffseg,end
    nbrden=6.806e28,end
    concd=d,12*1.0e5,end
    dcoef=d,equ,2,end
    qstrdr=d,const,0.0,end
    srcsd=d,const,0.0,srcpf,12*0.0,end
    difbcr=lawdep,encl,2
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    difbcl=lawdep,encl,3
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    surfa=1.8e-4,end
end of diffusion input
$
$
equation input
$
$ (1) Diffusivity of H in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960)]
y=3.728e-4*exp(-1315.8/temp),end
$
$ (2) Diffusivity of D in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960); divided by 1.414 for isotope effect]
y=2.636e-4*exp(-1315.8/temp),end
$
$ (3) Solubility of H,D in Pd
$ From measurements of Kizu et al.
y=1.511e23*exp(-5918./temp),end
$
end of equation input
$
$
table input
$ (1) Temperature history
0.0,865.,8.e5,865.,end
$ (2) Pressure history of D2 in Enclosure 5
0.0,1.20e-04,150.,1.20e-4,151.,2.41e-4,250.,2.41e-4,251.,6.06e-4,350.,6.06e-4
351.,1.30e-3,450.,1.30e-3,451.,2.53e-3,550.,2.53e-3,551.,7.08e-3,650.
7.08e-3,651.,1.45e-2,750.,1.45e-2,751.,2.63e-2,850.,2.63e-2,851.,6.51e-2
950.,6.51e-2,951.,0.116,1050.,0.116,1051.,0.297,1150.,0.297,1151.,0.76,
1250.,0.76,1251.,1.55,1350.,1.55,1351.,3.37,1900.,3.37,end
end of table input
$
$
control input
  time=0.0,end
  tstep=0.1,end
  timend=1450.0,end
  nprint=500,end
```

```
  itermx=9000,end
  delcmx=1.0e-7,end
  bump=1.e-3,end
  damp=0.7
  bound=4.0,end
  omega=1.3,end
end of control input
$
$
plot input
  nplot=1000,end
  plotseg=1,end
  plotencl=2,3,5,end
  dname=d,end
  ename=d2,end
  dplot=moblinv,sflux,end
  eplot=press,conv,diff,end
end of plot input
$
end of data
```

Problem 2ed: Co-permeation of H_2 and D_2 through 0.025-mm Pd at 870 K under Law-Dependent Boundary Conditions (Val-2ed)

```
title input
  Sample Problem #5d - Co-Permeation of D and H through Pd by K. Kizu,
  A. Pisarev and T. Tanabe, Journal of Nuclear Materials, 289 (2001) 291-302.
  Pd 0.025 mm, 870 K, H2, D2, and HD present, lawdep diffusion bc.
end of title input
$
main input
  dspcnme=h,d,end
  espcnme=h2,d2,hd,end
  segnds=12,end
  nbrencl=5,end
end of main input
$
enclosure input
$
start bdry,1,end
$ This is the background pressure source for both active chambers
    etemp=tabl,1,end
    esppres h2,1.0e-7,hd,2.0e-7,d2,1.0e-7,end
    outflow=nbrflwp,2,qflow,const,0.1,rencl,2
                      qflow,const,0.1,rencl,3,end
$
start func,2,end
$ This is the upstream chamber connecting to the membrane
    etemp=tabl,1,end
    esppres h2,0.063,hd,2.0e-7,d2,1.0e-7,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
    espcomb=hd,amu,3.0,eta,const,2.0
            h2,amu,2.0,pexp,0.5
            d2,amu,4.0,pexp,0.5,end
$
start func,3,end
$ This is the downstream chamber connected to the membrane
    etemp=tabl,1,end
    esppres h2,1.0e-20,hd,2.0e-20,d2,1.0e-20,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.005,end          $ Estimated volume
    espcomb=hd,amu,3.0,eta,const,2.0
            h2,amu,2.0,pexp,0.5
            d2,amu,4.0,pexp,0.5,end
$
start bdry,4,end
$ This is the gas sink representing the vacuum pumping system
    etemp=const,300.,end
    esppres h2,1.e-10,hd,1.e-10,d2,1.e-10,end
$
start bdry,5,end
$ This is the gas source with pre-programmed species pressures
    etemp=tabl,1,end
    esppres=h2,tabl,3,hd,const,1.0e-10,d2,tabl,2,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,2,end
end of enclosure input
```

```
$
thermal input
$  Segment 1  -  Pd film
start thermseg,end
    delx=0.0,10*2.5e-6,0.0,end
    tempd=12*300.0,end
    tcon=const,73.,end
    rhocp=const,2.932e6,end
    hsrc=const,0.0,srcpf,12*0.0,end
    htrbcl=stemp,tabl,1,end
    htrbcr=stemp,tabl,1,end
end of thermal input
$
$
diffusion input
$  Segment 1  -  Pd flim
start diffseg,end
    nbrden=6.806e28,end
    concd=h,12*1.e10,d,12*1.e10,end
    dcoef=h,equ,1,d,equ,2,end
    qstrdr=h,const,0.0,d,const,0.0,end
    srcsd=h,const,0.0,srcpf,12*0.0,d,const,0.0,srcpf,12*0.0,end
    difbcr=lawdep,encl,2
             dspc,h,h2,pexp,0.9297,solcon,equ,3
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    difbcl=lawdep,encl,3
             dspc,h,h2,pexp,0.9297,solcon,equ,3
             dspc,d,d2,pexp,0.9297,solcon,equ,3,end
    surfa=1.8e-4,end
end of diffusion input
$
$
equation input
$
$ (1) Diffusivity of H in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960)] Kept same as D2 for preservation of permeability
y=2.636e-4*exp(-1315.8/temp),end
$
$ (2) Diffusivity of D in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960); divided by 1.414 for isotope effect.
y=2.636e-4*exp(-1315.8/temp),end
$
$ (3) Solubility of H/D in Pd based on measurements of Kizu et al.
y=9.355e22*exp(-5918./temp),end
$
end of equation input
$
$
table input
$ (1) Temperature history
0.0,870.,8.e5,870.,end
$ (2) Pressure history of D2 in Enclosure 5
0.,1.8421e-4,150.,1.8421e-4,151.,1.0e-3,250.,1.0e-3,251.,3.0e-3,350.
3.0e-3,351.,0.009,450.,0.009,451.,0.027,550.,0.027,551.
0.081,650.,0.081,651.,0.243,750.,0.243,751.,0.729,1.e6,0.729,end
$ (3) Pressure history of H2 in Enclosure 5
0.0,0.063,1000.,0.063,end
```

```
end of table input
$
$
control input
  time=0.0,end
  tstep=0.1,end
  timend=801.0,end
  nprint=500,end
  itermx=1000,end
  delcmx=1.0e-6,end
  bump=1.e-3,end
  damp=0.7
  bound=9.0,end
  omega=0.9,end
end of control input
$
$
plot input
  nplot=1000,end
  plotseg=1,end
  plotencl=2,3,5,end
  dname=h,d,end
  ename=h2,hd,d2,end
  dplot=moblinv,sflux,end
  eplot=press,conv,diff,end
end of plot input
$
end of data
```

Problem 2ee: Co-permeation of H_2 and D_2 through 0.025-mm Pd at 870 K under Recombination-Limited Boundary Conditions (Val-2ee)

```
title input
  Sample Problem #5e - Co-Permeation of D and H throu Pd by K. Kizu,
  A. Pisarev and T. Tanabe, Journal of Nuclear Materials, 289 (2001) 291-302.
  Pd 0.025 mm, 870 K, H2, D2, and HD present, ratedep diffusion bc
end of title input
$
main input
  dspcnme=h,d,end
  espcnme=h2,d2,hd,end
  segnds=12,end
  nbrencl=5,end
end of main input
$
enclosure input
$
start bdry,1,end
$ This is the background pressure source for both active chambers
    etemp=tabl,1,end
    esppres h2,1.0,hd,1.0,d2,1.0,end
    outflow=nbrflwp,2,qflow,const,1.e-8,rencl,2
                      qflow,const,1.e-8,rencl,3,end
$
start func,2,end
$ This is the upstream chamber connecting to the membrane
    etemp=tabl,1,end
    esppres h2,0.063,hd,2.0e-7,d2,1.0e-7,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.05,end          $ Estimated volume
$
start func,3,end
$ This is the downstream chamber connected to the membrane
    etemp=tabl,1,end
    esppres h2,1.0e-7,hd,2.0e-7,d2,1.0e-7,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,4,end
    evol=0.05,end          $ Estimated volume
$
start bdry,4,end
$ This is the gas sink representing the vacuum pumping system
    etemp=tabl,1,end
    esppres h2,1.e-10,hd,1.e-10,d2,1.e-10,end
$
start bdry,5,end
$ This is the gas source with pre-programmed species pressures
    etemp=tabl,1,end
    esppres=h2,const,0.063,hd,const,1.0e-10,d2,tabl,2,end
    outflow=nbrflwp,1,qflow,const,0.1,rencl,2,end
end of enclosure input
$
thermal input
$  Segment 1  -  Pd film
start thermseg,end
    delx=0.0,10*2.5e-6,0.0,end
    tempd=12*300.0,end
```

```
    tcon=const,73.,end
    rhocp=const,2.932e6,end
    hsrc=const,0.0,srcpf,12*0.0,end
    htrbcl=stemp,tabl,1,end
    htrbcr=stemp,tabl,1,end
end of thermal input
$
diffusion input
$  Segment 1  -  Pd flim
start diffseg,end
    nbrden=6.806e28,end
    concd=h,12*1.0,d,12*1.0,end
    dcoef=h,equ,1,d,equ,2,end
    qstrdr=h,const,0.0,d,const,0.0,end
    srcsd=h,const,0.0,srcpf,12*0.0,d,const,0.0,srcpf,12*0.0,end
    difbcl=ratedep,encl,2
           spc,h
             exch,h2,ksubd,equ,4
                  h,ksubr,equ,7
             exch,hd,ksubd,equ,5
                  d,ksubr,equ,9
           spc,d
             exch,d2,ksubd,equ,6
                  d,ksubr,equ,8
             exch,hd,ksubd,equ,5
                  h,ksubr,equ,9,end
    difbcr=ratedep,encl,3
           spc,h
             exch,h2,ksubd,equ,4
                  h,ksubr,equ,7
             exch,hd,ksubd,equ,5
                  d,ksubr,equ,9
           spc,d
             exch,d2,ksubd,equ,6
                  d,ksubr,equ,8
             exch,hd,ksubd,equ,5
                  h,ksubr,equ,9,end
    surfa=1.8e-4,end
end of diffusion input
$
equation input
$
$ (1) Diffusivity of H in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960)]
y=3.728e-4*exp(-1315.8/temp),end
$
$ (2) Diffusivity of D in Pd [O. M. Katz & E. A. Gulbransen,Rev. Sci. Instr.,
$ 31, 615-617 (1960)]
y=2.636e-4*exp(-1315.8/temp),end
$
$ (3) Solubility of D in Pd based on measurements of Kizu et al.
y=9.355e22*exp(-5918./temp),end
$
$ (4) Dissociation coefficient for H2
y=2.1898e22/sqrt(2.*temp)/sqrt(2.),end
$
$ (5) Dissociation coefficient for HD
```

```
y=2.1898e22/sqrt(2.*temp)/sqrt(3.),end
$
$ (6) Dissociation coefficient for D2
y=2.1898e22/sqrt(2.*temp)/2.,end
$
$ (7) Recombination coefficient H2
y=2.502e-24*exp(-11836./temp)/sqrt(2.*temp),end
$
$ (8) Recombination coefficient D2
y=2.502e-24*exp(-11836./temp)/sqrt(3.*temp),end
$ (9) Recombination coefficient HD
y=5.004e-24*exp(-11836./temp)/sqrt(4.*temp),end
$
$ (10) Solubility of H in Pd based on measurements of Kizu et al.
y=9.355e22*exp(-5918./temp),end
$
end of equation input
$
table input
$ (1) Temperature history
0.0,870.,8.e5,870.,end
$ (2) Pressure history of D2 in Enclosure 5
0.,1.8421e-4,110.,1.8421e-4,111.,1.0e-3,210.,1.0e-3,211.,3.0e-3,310.
3.0e-3,311.,0.009,410.,0.009,411.,0.027,510.,0.027,511.
0.081,610.,0.081,611.,0.243,710.,0.243,711.,0.729,1.e6,0.729,end
$ (3) Pressure history of H2 in Enclosure 5
0.0,0.063,1000.,0.063,end
end of table input
$
control input
  time=0.0,end
  tstep=0.1,end
  timend=810.0,end
  nprint=1000,end
  itermx=1000,end
  delcmx=1.0e-6,end
  bump=1.e-3,end
  damp=0.7
  bound=4.0,end
  omega=0.9,end
end of control input
$
plot input
  nplot=1000,end
  plotseg=1,end
  plotencl=2,3,5,end
  dname=h,d,end
  ename=h2,hd,d2,end
  dplot=moblinv,sflux,sconc,end
  eplot=press,conv,diff,end
end of plot input
$
end of data
```