

SCIENTIFIC SOFTWARE & MODELLING SOLUTIONS

AMBER 5.4 Verification Summary



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Quintessa Limited
The Hub • 14 Station Road
Henley-on-Thames • Oxfordshire RG9 1AY
United Kingdom
Phone: +44 (0)1491 630052
Fax: +44 (0)1491 636247
email: amber@quintessa.org
www.quintessa.org/amber/

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1 Introduction

The AMBER compartment modelling code is a general-purpose tool. It allows the development of compartment models, and calculation of their solutions, for a wide range of situations. Details of AMBER and its use are provided in Quintessa (2010a, b, c and d).

The verification of such a computer tool is essentially a matter of demonstrating that the code does what it claims. That is, the models are solved correctly in accordance with what has been specified. The verification of the models themselves, as opposed to the computer code, is the responsibility of the model developer who uses AMBER.

However, in the process of verifying specific models, users are implicitly verifying the correct functioning of the underlying tool. In this way, every application of AMBER builds confidence in the tool itself. This is particularly true when intercomparisons with other codes are performed and when checks against analytic solutions are made.

Some published applications of AMBER involving such intercomparisons are discussed in Section 2.

In addition to the ongoing use of the tool, it is useful to have a set of test cases specifically developed to check the correct functioning of the code. Various tests have been developed. This document brings together a set of these tests and reports on their application to the 5.4 version of AMBER (Quintessa, 2010a). This report is accompanied by electronic versions of the AMBER case files, which are referred to in the documentation of each test.

Although the tests described here are primarily designed to check that the correct solution is calculated, they incidentally check the correct functioning of the graphical user interface. This, together with the tests performed when a new graphical element is added, or when a change is made, give confidence in the correct functioning of the user interface aspects of AMBER.

The tests described here are as follows.

- ▲ Some simple cases with known solutions that have been used throughout AMBER's development (Section 3).
 - ▲ The NEA PSAG Level 1B exercise, which checks the deterministic and probabilistic functioning of AMBER against the documented results from a number of participant members of the PSAG group (Section 4).
 - ▲ A comparison with a solubility-limited source term model, developed by AEA Technology for Nirex (Section 5).
 - ▲ A comparison with a spreadsheet calculation for a case involving a Langmuir Availability scheme (Section 6).
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- ▲ A case using all of the available probability distributions to check that sensible values are generated, by comparing calculated statistics with the known true values (Section 7).
- ▲ Section 8 describes the results of cases used to test that sampling is properly random and that correlations are appropriately generated when specified.

These cases all perform well and give confidence in the correct functioning of the code.

In addition, Section 9 describes the results of ‘pressure testing’ of the code and solvers to determine some of the practical limits for aspects including transfer rates, number handling, contaminants and transfers. Section 10 summarises the testing undertaken for the new features and bug fixes in AMBER 5.4.

Brief conclusions are presented in Section 11, whilst references are provided at the end of the report.

2 Published Applications

AMBER has been applied in many projects. The AMBER Example, Users and References document (Quintessa, 2010c) includes a list of publications that describe assessments in which AMBER has been applied. The following is a short selection of those that include comparisons with other codes.

As part of SKI's review of SKB's calculations for the SFR 1 repository for low and intermediate level waste, AMBER was used to undertake an exploration of some of the important issues (Maul and Robinson, 2002). As well as demonstrating the applicability of AMBER in an overall performance assessment, the calculations include direct comparisons with SKB calculations. Given the slightly different modelling assumptions that were made, the results agree well.

In addition, SKI and SSI have undertaken an intercomparison between AMBER and Ecolego to give confidence in their application to total-system performance assessment (PA) studies for deep repositories and to further review SKB's SR 97 calculations (Maul et al., 2003 and 2004). The studies compared the results for near-field, geosphere and biosphere implementations, considering both deterministic and probabilistic calculations. The studies demonstrated good agreement between the two codes.

SKB have used AMBER as the benchmark against which to test their Tensit simulation tool (Jones et al., 2004). The study demonstrates excellent agreement between the two codes.

AMBER was successfully used in the Vault Test Case of the IAEA's ISAM programme to model the migration and fate of liquid and solid releases from a near-surface radioactive waste repository (IAEA, 2003a). The results obtained from AMBER were in agreement with those obtained using other internationally recognised codes.

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AMBER was used in support of the IAEA's BIOMASS programme (IAEA, 2003b). The results for Example Reference Biospheres (ERBs) 2A and 2B were obtained following their implementation in AMBER. Very close agreement was achieved when the AMBER results for ERB 2A were compared with the results achieved following its implementation in a different software package.

The performance of AMBER was evaluated against the Pacific Northwest Laboratory's MEPAS code and Andra's AQUABIOS code in assessing the environmental impact of non-radioactive contaminants (Côme et al., 2004, ANDRA, 2003). The project demonstrated close agreement between AMBER and the other codes.

Models developed using AMBER have been compared against other models in BIOMOV5 II. QuantiSci (now Envirosc Consulting Limited) developed an AMBER model for the C-14 release to a lake scenario (BIOMOV5, 1996a), whilst Ciemat (Spain) developed models for the Complementary Studies (BIOMOV5, 1996b) and lysimeter (BIOMOV5, 1996c) exercises.

In work for the FSA (formerly MAFF), AMBER cases were developed to reproduce earlier results produced by the MAFF H3 and C14 STAR codes (Watkins et al., 1998). The results were reproduced precisely.

AMBER models, in conjunction with models from IPSN and ANDRA (France) have been used in an IAEA study to derive activity limits for the near-surface disposal of radioactive waste (IAEA, 2003c).

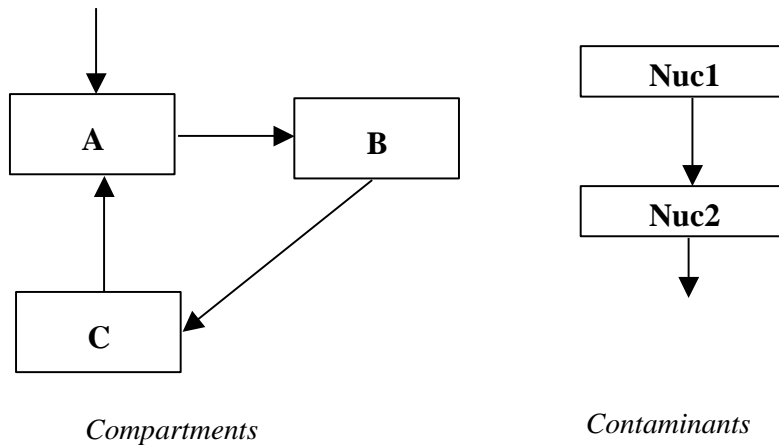
In an application to subsurface transport, AMBER models have also been used by an MSc student to represent the migration of contaminants in an aquifer and the results successfully compared against analytical solutions (Scott, 1998).

3 Simple Test Cases

3.1 SN2

This case is a simple system with three compartments and two contaminants (see Figure 3.1-1). The transfer rates are piecewise constant. Results (amount of each contaminant in each compartment against time) were calculated with the SPADE code (a general differential equation solver) (Williams and Woods, 1994) and compared to those obtained using AMBER.

Figure 3.1-1: Structure of SN2



Nuc1 decays at a rate of 1E-4 per year and Nuc2 at a rate of 1E-2 per year.

The source to A is for Nuc1 only. It is zero except for two time intervals: from 0 to 10 years it is 1 mol/y, and from 30 to 50 years it is 2 mol/y.

This test case is implemented in *SN2.cse*. The initial transfer rates are given in the Table 3.1-1. After 40 years they all fall by a factor of 100.

Table 3.1-1: Initial Transfer Rates for SN2

Transfer		Initial Transfer Rate (per year)	
From	To	Nuc1	Nuc2
A	B	0.01	0.001
B	C	0.001	0.1
C	A	0.1	0.1

Results are calculated at 10, 20, 30, 40, 50 and 100 years.

The 10 and 100 year results are quoted as representative in Table 3.1-2. Differences from the SPADE results are shown by highlighting the digits that differ. Results (amounts in moles) with both AMBER's Laplace and time-stepping solver are compared to 6 significant figures. The agreement is very good throughout.

Table 3.1-2: Comparison of SN2 Results with SPADE (moles)

Compartment	Contaminant	Time	SPADE	AMBER with Laplace Solver	AMBER with Time-step Solver
A	Nuc1	10	9.51191	9.51191	9.51191
A	Nuc2	10	0.00466821	0.00466821	0.00466821
B	Nuc1	10	0.481807	0.481807	0.481807
B	Nuc2	10	0.000137848	0.000137849	0.000137849
C	Nuc1	10	0.00128303	0.00128305	0.00128305
C	Nuc2	10	2.97304E-5	2.97307E-5	2.97310E-5
A	Nuc1	100	45.5501	45.5501	45.5501
A	Nuc2	100	0.220230	0.220230	0.220229
B	Nuc1	100	4.09113	4.09113	4.09114
B	Nuc2	100	0.0188336	0.0188336	0.0188335
C	Nuc1	100	0.0249555	0.0249555	0.0249547
C	Nuc2	100	0.00142203	0.00142203	0.00142206

3.2 SN5

SN5 tests a simple case with non-depleting transfers and local decay rates, the structure is illustrated in Figure 3.2-1.

Nuc1 decays at a rate of 0.01 per year in compartment A only. The transfers are both non-depleting and have a rate of 1 per year. Thus, B calculates the integral of A; and C calculates the integral of B. Initially, there is 1 mole of Nuc1 in A.

The solution is simply:

$$A = e^{-\lambda t}$$

$$B = \frac{1 - e^{-\lambda t}}{\lambda}$$

$$C = \frac{t}{\lambda} - \frac{1 - e^{-\lambda t}}{\lambda^2}$$

where λ is the decay rate.

This test case is implemented in *SN5.cse*. The Laplace solver and time-step solver have both been used to calculate the amount of Nuc1 (moles) in each compartment as a function of time. The results are compared with an analytical solution in Table 3.2-1. The agreement is very good throughout.

Figure 3.2-1: Structure of SN5

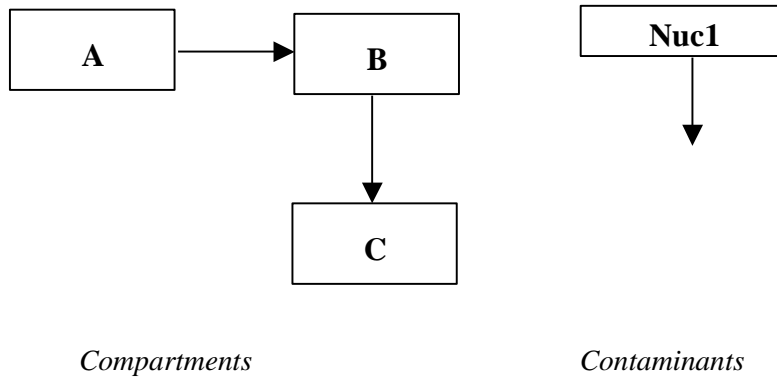


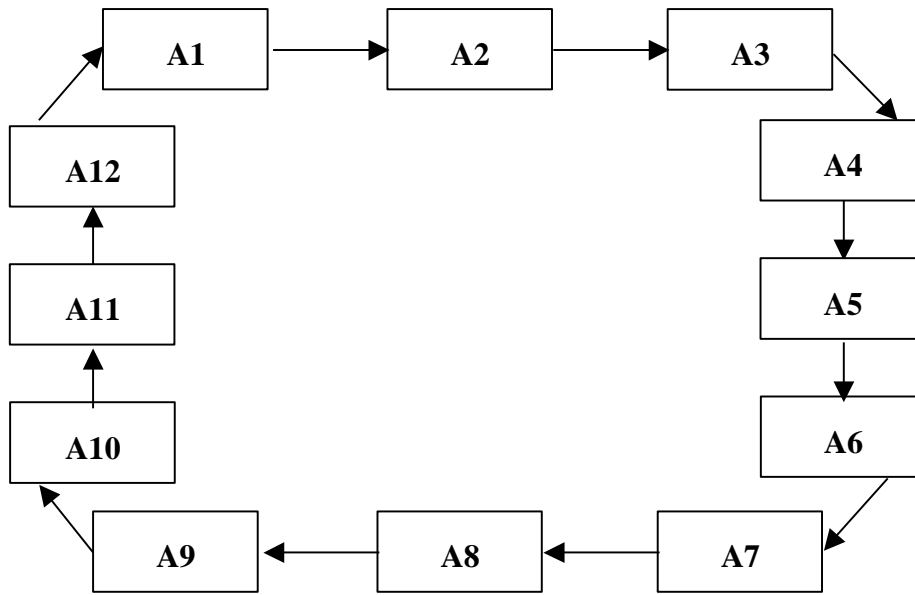
Table 3.2-1: Results of SN5 (moles)

Time	Compartment	Analytic	Laplace Solver	Time-step Solver
0.01	A	0.999900	0.999900	0.999900
0.01	B	0.00999950	0.00999950	0.00999949
0.01	C	4.99983E-5	4.99983E-5	5.05133E-5
10	A	0.904837	0.904837	0.904837
10	B	9.51626	9.51626	9.51626
10	C	48.3742	48.3742	48.3742
100	A	0.367879	0.367879	0.367872
100	B	63.2121	63.2121	63.2128
100	C	3678.79	3678.79	3678.72
1000	A	4.53999E-5	4.53999E-5	4.61771E-5
1000	B	99.9955	99.9955	99.9954
1000	C	90000.5	90000.5	90000.5

3.3 SN7

SN7 is a case with a loop of compartments with identical transfer rates and a non-decaying contaminant. A general analytic solution can be found for any number of compartments. Here, 12 have been used (see Figure 3.3-1).

Figure 3.3-1: Structure of SN7



All the transfer rates are 0.1 per year and the initial amounts are: 1 mol in A1, A2, A4, A6, A7 and A10; zero elsewhere.

The analytic result for a general system with N compartments in a loop and a transfer rate of μ is derived as follows.

The equation for the amount in compartment n is:

$$\frac{dA_n}{dt} = \mu A_n - \mu A_{n-1}$$

where A_0 and A_N are equivalent. We look for eigen-solutions with:

$$A_n(t) = E_n e^{-\gamma t}$$

from the governing equation it is clear that:

$$E_n = \frac{\mu}{\mu - \gamma} E_{n-1}$$

and the loop symmetry gives:

$$\left(\frac{\mu}{\mu - \gamma} \right)^N = 1.$$

The eigen-values are therefore given by:

$$\gamma^{(k)} = \mu(1 - e^{-2\pi i k / N})$$

with corresponding eigen-solutions:

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$$E_n^{(k)} = e^{2\pi i.k.n/N} .$$

This then leads to the solution:

$$A_n(t) = \sum_{k=1}^N \alpha^{(k)} E_n^{(k)} e^{-\gamma^{(k)}t} ,$$

where:

$$\alpha^{(k)} = \frac{1}{N} \sum_{n=1}^N A_n(0) E_n^{(k)} .$$

From this, results at 20, 40, 60, 80 and 100 have been calculated. These are presented in Table 3.3-1.

Table 3.3-1: Analytical Results for SN7

Compartment	Amounts (moles)				
	t=20	t=40	t=60	t=80	t=100
A1	0.331448	0.393231	0.493590	0.545518	0.541057
A2	0.500565	0.382391	0.450256	0.521544	0.542698
A3	0.578488	0.421262	0.422288	0.489768	0.532723
A4	0.598713	0.483640	0.421521	0.460279	0.513205
A5	0.544824	0.530970	0.445906	0.443184	0.489534
A6	0.533186	0.548898	0.481307	0.443560	0.468849
A7	0.634764	0.561520	0.514184	0.459365	0.457322
A8	0.647070	0.584441	0.540759	0.484075	0.457839
A9	0.491510	0.589493	0.561193	0.510966	0.469434
A10	0.419087	0.556907	0.570820	0.534847	0.488415
A11	0.400650	0.503189	0.562832	0.551199	0.509930
A12	0.319694	0.444059	0.535343	0.555695	0.528994

The test case is implemented in AMBER in *SN7.cse* and the results, using the time-step solver, are shown in Table 3.3-2. The digits that disagree are highlighted.

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Table 3.3-2: AMBER Results for SN7

Compartment	Amounts (moles)				
	t=20	t=40	t=60	t=80	t=100
A1	0.331439	0.393228	0.493591	0.545508	0.541053
A2	0.500576	0.382384	0.450256	0.521533	0.542690
A3	0.578493	0.421278	0.422296	0.489764	0.532711
A4	0.598697	0.483641	0.421539	0.460290	0.513196
A5	0.544834	0.530961	0.445919	0.443209	0.489540
A6	0.533181	0.548888	0.481297	0.443584	0.468872
A7	0.634769	0.561518	0.514158	0.459366	0.457353
A8	0.647075	0.584458	0.540749	0.484052	0.457857
A9	0.491499	0.589501	0.561213	0.510944	0.469429
A10	0.419083	0.556886	0.570833	0.534847	0.488397
A11	0.400666	0.503184	0.562819	0.551208	0.509914
A12	0.319687	0.444074	0.535331	0.555695	0.528988

The agreement is generally to 3-4 significant figures, with no deterioration for larger times.

As an experiment, an extra disconnected transfer was added with a faster transfer rate (10). This causes AMBER to take shorter time-steps, at least initially. This change is implemented in *SN7(Extra).cse* and the calculated results are shown in Table 3.3-3.

Table 3.3-3: AMBER Results for SN7 with a Faster Transfer Rate Added

Compartment	Amounts (moles)				
	t=20	t=40	t=60	t=80	t=100
A1	0.331440	0.393228	0.493590	0.545509	0.541053
A2	0.500576	0.382384	0.450256	0.521533	0.542689
A3	0.578492	0.421277	0.422296	0.489764	0.532710
A4	0.598697	0.483641	0.421539	0.460289	0.513196
A5	0.544835	0.530961	0.445919	0.443208	0.489540
A6	0.533180	0.548888	0.481297	0.443583	0.468873
A7	0.634770	0.561518	0.514159	0.459366	0.457353
A8	0.647075	0.584457	0.540749	0.484053	0.457857
A9	0.491499	0.589500	0.561212	0.510945	0.469429
A10	0.419083	0.556887	0.570833	0.534847	0.488397
A11	0.400666	0.503184	0.562820	0.551207	0.509914
A12	0.319687	0.444073	0.535331	0.555695	0.528988

These results are very similar to those presented in Table 3.3-2, with only small differences at the sixth significant figure.

4 Level 1B

PSAG Level 1B has a biosphere model with multiple transfers, compartments and contaminants. Transfer rates are specified as formulae. The exercise was organised by the NEA PSAG (Probabilistic Safety Assessment Group) (NEA, 1993).

Deterministic and probabilistic results are given.

4.1 Deterministic

Initially, a precise match could not be obtained. Further investigation revealed three small errors in the printed Level1B report that explain this. The errors are: in equation 16, $\tan \theta$ should be $\sin \theta$; and in equations 37 and 38 where the denominators should match the food type.

Having corrected these, the rates quoted in Table B5 of NEA (1993) are matched.

Table D1 of NEA (1993) gives the Bq inventories at a number of times. The participants generally agree. This test case is implemented in *Level1B.cse* and the deterministic results are generated by calculating *Level1B.cse* with the 'Best Estimates' sampling option selected

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in the Calculate dialogue. The AMBER results are compared against the AEAT results using MASCOT in Table 4.1-1, as this is a semi-analytic solution and should be the most accurate and can be directly compared.

Table 4.1-1: Comparison of AMBER and Mascot Amounts for Level1B

Time	AMBER: Amount (Bq)			MASCOT: Amount (Bq)		
	1	1000	100000	1	1000	100000
Nuclide	Compartment: Water					
C14	4.67E+3	2.71E+3	2.20E-3	4.66E+3	2.70E+3	2.19E-3
U235	3.42E+0	9.69E+0	7.56E+0	3.41E+0	9.67E+0	7.55E+0
Pa231	7.25E-5	2.32E-1	6.58E+0	7.24E-5	2.32E-1	6.57E+0
Ac227	1.14E-6	2.16E-1	6.19E+0	1.14E-6	2.16E-1	6.18E+0
Nuclide	Compartment: Sediment					
C14	1.20E+3	3.87E+3	3.14E-3	1.20E+3	3.86E+3	3.13E-3
U235	8.70E-1	1.08E+1	8.46E+0	8.68E-1	1.08E+1	8.45E+0
Pa231	1.63E-5	2.62E-1	7.48E+0	1.62E-5	2.62E-1	7.46E+0
Ac227	2.30E-7	2.08E-1	6.00E+0	2.30E-7	2.08E-1	5.99E+0
Nuclide	Compartment: TopSoil					
C14	1.80E+6	2.76E+9	5.11E+3	1.81E+6	2.76E+9	5.11E+3
U235	4.64E+2	4.88E+7	5.66E+7	4.64E+2	4.88E+7	5.66E+7
Pa231	9.78E-3	1.24E+6	4.93E+7	9.78E-3	1.24E+6	4.93E+7
Ac227	1.54E-4	1.14E+6	4.62E+7	1.54E-4	1.14E+6	4.63E+7
Nuclide	Compartment: DeepSoil					
C14	2.21E+8	1.21E+11	2.24E+5	2.21E+8	1.21E+11	2.24E+5
U235	1.63E+5	1.06E+8	1.13E+8	1.63E+5	1.06E+8	1.13E+8
Pa231	3.45E+0	2.00E+6	6.81E+7	3.45E+0	1.80E+6	6.82E+7
Ac227	5.42E-2	2.00E+6	7.12E+7	5.42E-2	2.00E+6	7.12E+7

The only significantly different result is for Pa-231 in Deep Soil at 1000 years. Other participants give the result as 2.00E+6, in agreement with AMBER, so it is supposed that the quoted result is probably erroneous.

Given the good match seen here, the dose results should match well. A full set of results is given in Section D2 of NEA (1993). This is confirmed by a few spot checks. In Table 4.1-2 the U-235 results are compared in detail.

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Table 4.1-2: Comparison of AMBER and Mascot Dose Rates for Level1B

Time	AMBER: Dose (Sv/y)			MASCOT: Dose (Sv/y)		
	1	1000	100000	1	1000	100000
Water	5.1E-12	1.4E-11	1.1E-11	5.1E-12	1.4E-11	1.1E-11
Fish	1.1E-12	3.1E-12	2.4E-12	1.1E-12	3.1E-12	2.4E-12
Grain	1.5E-13	1.8E-9	2.1E-9	1.5E-13	1.8E-9	2.1E-9
Meat	7.0E-12	1.6E-8	1.8E-8	7.0E-12	1.6E-8	1.8E-8
Milk	4.5E-14	9.9E-11	1.2E-10	4.5E-14	9.9E-11	1.1E-10
Dust	1.9E-14	2.0E-9	2.3E-9	1.9E-14	2.0E-9	2.3E-9
External	3.9E-14	4.1E-9	4.8E-9	4.0E-14	4.2E-9	4.8E-9

4.2 Stochastic

For stochastic results, a precise match is not expected. Most participants used 1000 samples, so the AMBER results are also generated using 1000 samples with the 'Full' Sampling option selected in the Calculate dialogue and a seed of 987654321.

Table D3 of NEA (1993) gives the results for C14 total dose and U235 chain total dose.

The mean results obtained with AMBER are compared against the range of means obtained by participants using Monte Carlo analysis.

Table 4.2-1: Mean Stochastic Results for Level1B

Time	AMBER: Total dose (Sv/y)		Participants: Total dose (Sv/y)	
	C14	U235 Chain	C14	U235 Chain
1	1.53E-7	2.30E-11	1.3E-7 to 1.5E-7	2.1E-11 to 2.3E-11
3	6.92E-7	2.95E-11	6.1E-7 to 7.0E-7	2.8E-11 to 3.0E-11
10	2.79E-6	8.94E-11	2.5E-6 to 2.8E-6	8.1E-11 to 9.0E-11
30	8.70E-6	4.36E-10	7.8E-6 to 8.7E-6	4.0E-10 to 4.4E-10
100	2.79E-5	2.67E-9	2.5E-5 to 2.8E-5	2.6E-9 to 2.7E-9
300	7.15E-5	1.57E-8	6.5E-5 to 7.1E-5	1.5E-8 to 1.6E-8
1000	1.40E-4	1.29E-7	1.3E-4 to 1.4E-4	1.3E-7 to 1.4E-7
3000	1.15E-4	8.92E-7	1.1E-4 to 1.1E-4	8.8E-7 to 9.5E-7
10000	2.56E-5	5.96E-6	2.5E-5 to 2.7E-5	6.0E-6 to 6.5E-6
30000	1.12E-6	2.03E-5	1.1E-6 to 1.2E-6	2.1E-5 to 2.3E-5
100000	9.23E-11	2.05E-5	7.9E-11 to 1.0E-10	2.2E-5 to 2.4E-5
300000	*	3.12E-6	*	3.3E-6 to 4.2E-6
1000000	*	2.03E-7	*	1.7E-7 to 3.0E-7

*Result very small

The AMBER results for both C-14 and the U-235 chain agree well with the range reported by the PSACOIN Level 1B participants.

5 Solubility Limited Case

In this section, a comparison is made with a published report on a solubility limited source model developed for Nirex and other UK organisations (Robinson et al, 1988), which is referred to here by its reference number, R11854.

R11854 reports on a solubility limited source term model.

The results are calculated for 55 nuclides, including stable species.

R11854 omits to give the U-233 inventory, which has been set to give the same peak toxicity for Th-229.

5.1 Toxicity

R11854 gives maximum near-field Toxicity and Time of Occurrence for each nuclide where the maximum is more than 0.1.

AMBER 5.4 Verification Summary

This test case is implemented in *R11854.cse* and the results can be directly compared with those from R11854 (see Table 5.1-1).

Table 5.1-1: Comparison of AMBER Maximum Toxicity with R11854

Nuclide	AMBER		R11854	
	Maximum Toxicity	Time of Occurrence	Maximum Toxicity	Time of Occurrence
C14	2.72E+1	300	2.73E+1	300
Se79	1.05E+1	300	1.05E+1	300
Sr90	9.70E+3	300	9.70E+3	300
Nb93m	3.47E+3	300	3.48E+3	300
Nb94	2.22E+4	300	2.22E+4	300
Tc99	3.17E-1	383.597	3.17E-1	300
Sn126	3.33E+1	300	3.33E+1	300
I129	5.35E+1	300	5.36E+1	300
Cs135	4.41E+0	300	4.42E+0	300
Cs137	8.66E+3	300	8.67E+3	300
Pb210	7.14E+4	300	7.16E+4	300
Ra226	2.52E+3	300	2.53E+3	300
Ac227	2.87E+1	300000	2.90E+1	3E+5
Th229	7.31E+1	34756	7.31e+1	4E+4
Th230	2.21E+0	406040	2.20E+0	5E+5
Pa231	2.02E+1	300000	2.04E+1	3E+5
Np237	1.68E+1	3000	1.68E+1	3E+3
Pu238	6.94E-1	300	6.73E-1	300
Pu239	1.33E+1	40944.8	1.33E+1	5E+4
Pu240	9.28E+0	300	8.96E+0	300
Pu242	7.32E-1	269554*	6.57E-1	3E+5
Am241	1.28E+3	300	1.28E+3	300
Am242m	9.64E-1	300	7.97E-1	300
Am243	4.11E+0	1311.13*	3.84E+0	1E+3

Note: * These values would round to the value reported for R11854 and are therefore considered consistent.

5.2 Effective Leach Rate

R11854 gives initial and maximum effective leach rate (to 10^6 years) for each element. These can be directly compared (see Table 5.2-1).

Table 5.2-1: Comparison of AMBER Leach Rates with R11854 (y^{-1})

Element	AMBER		R11854	
	Initial Leach Rate	Maximum Leach Rate	Initial Leach Rate	Maximum Leach Rate
H	8.0E-3	8.0E-3	Not given	Not given
C	8.1E-4	7.7E-3	8.1E-4	7.7E-3
Ni	8.2E-9	8.3E-9	8.2E-9	8.3E-9
Se	7.7E-3	7.7E-3	7.7E-3	7.7E-3
Sr	1.6E-3	1.6E-3	1.6E-3	1.6E-3
Zr	1.3E-7	1.5E-7	1.3E-7	1.5E-7
Nb	7.7E-3	7.7E-3	7.7E-3	7.7E-3
Tc	1.5E-5	2.0E-4	1.5E-5	2.0E-4
Sn	7.7E-3	7.7E-3	7.7E-3	7.7E-3
I	7.7E-3	7.7E-3	7.7E-3	7.7E-3
Cs	1.6E-3	1.6E-3	1.6E-3	1.6E-3
Sm	2.7E-9	2.7E-9	2.7E-9	2.7E-9
Pb	7.7E-3	7.7E-3	7.7E-3	7.7E-3
Ra	1.6E-3	1.6E-3	1.6E-3	1.6E-3
Ac	2.0E-4	2.0E-4	2.0E-4	2.0E-4
Th	2.0E-6	2.0E-6	2.0E-6	2.0E-6
Pa	2.0E-4	2.0E-4	2.0E-4	2.0E-4
U	2.3E-13	2.3E-13	2.3E-13	2.3E-13
Np	2.0E-6	2.0E-6	2.0E-6	2.0E-6
Pu	7.5E-9	2.0E-6	7.3E-9	2.0E-6
Am	4.5E-7	2.0E-6	4.5E-7	2.0E-6
Cm	2.0E-6	2.0E-6	2.0E-6	2.0E-6

5.3 Result of Comparison

The comparison with R11854 gives generally good agreement. The discrepancies could be caused by data errors in the original report or by numerical issues. None are serious enough to cause any concern.

6 Langmuir Availability Test

In order to test the correct functioning of the Langmuir Availability scheme, two cases have been run.

The first uses a limiting case to give an analytic result. The second compares the results of a shared scheme with a separately coded solution (using a larger number of simple timesteps).

6.1 Simple Limiting Case

For a single compartment and contaminant, with a source, Langmuir-controlled loss rate and decay constant, the equation for the amount is:

$$\frac{dA}{dt} = -\lambda A + s - \mu A \frac{A + \alpha}{A + \beta}.$$

In the limit as $\beta \rightarrow 0$ this becomes simply:

$$\frac{dA}{dt} = -(\lambda + \mu)A + s - \mu\alpha.$$

In the case where $s = \mu\alpha$, the solution is simply:

$$A = A_0 e^{-(\lambda + \mu)t},$$

where A_0 is the initial amount.

Here $A_0 = 1$, $\lambda = 0.001$, $\mu = 0.01$, $\alpha = 0.5$ and $\beta = 10^{-20}$. The last of these is chosen to be as close to zero as possible (AMBER does not allow a zero value). A good match is expected for all times when $A \gg \beta$.

The test case is implemented in *SimpleLimitingCase.cse* and the results can be directly compared with the analytical solution (see Table 6.1-1). As can be seen, the match is very good throughout.

Table 6.1-1: AMBER and Analytical Results for Simple Langmuir Solutions (moles)

Time	AMBER	Analytic	Ratio
0	1.000E+0	1.000E+0	1.000
1	9.891E-1	9.891E-1	1.000
2	9.782E-1	9.782E-1	1.000
5	9.465E-1	9.465E-1	1.000
10	8.958E-1	8.958E-1	1.000
20	8.025E-1	8.025E-1	1.000
50	5.770E-1	5.769E-1	1.000
100	3.329E-1	3.329E-1	1.000
200	1.108E-1	1.108E-1	1.000
500	4.086E-3	4.087E-3	1.000
1000	1.669E-5	1.670E-5	0.999
1200	1.849E-6	1.850E-6	0.999
1500	6.808E-8	6.830E-8	0.997
2000	2.761E-10	2.790E-10	0.990

6.2 Shared Langmuir Case

In this test, there are two contaminants with a shared Langmuir scheme. The two have different decay rates and there are different sources. The first contaminant decays to the second. The equations solved are:

$$\frac{dA}{dt} = -\lambda_A A + s_A - \mu_A A \frac{A+B+\alpha}{A+B+\beta}$$

$$\frac{dB}{dt} = \lambda_A A - \lambda_B B + s_B - \mu_B B \frac{A+B+\alpha}{A+B+\beta}$$

In the absence of analytic results, a small spreadsheet has been created that solves these equations using small explicit steps.

The data used is as follows. Here $A_0 = 1$, $B_0 = 2$, $\lambda_A = 0.001$, $\lambda_B = 0.003$, $\mu_A = 0.01$, $\mu_B = 0.005$, $s_A = 0.002$, $s_B = 0.001$, $\alpha = 0.5$ and $\beta = 1$.

The results tend to a steady state where the source balances the decay and loss rates.

The spreadsheet results are calculated with a step of 0.1. Each step consists of an explicit forward step from which an approximate average value over the step is obtained. This is then used for the full step.

AMBER 5.4 Verification Summary

This test case is implemented in *SharedLangmuirCase.cse* and the results can be directly compared with the analytical solution (see Table 6.2-1). The agreement obtained is excellent, confirming the correct behaviour of the Langmuir calculation.

Table 6.2-1: AMBER and Analytical Results for Shared Langmuir Schemes (moles)

Time	AMBER		Analytic		Ratio	
	A	B	A	B	A	B
0	1.00000	2.00000	1.00000	2.00000	1.00000	1.00000
1	0.99229	1.98730	0.99229	1.98730	1.00000	1.00000
2	0.98466	1.97468	0.98466	1.97468	1.00000	1.00000
5	0.96226	1.93739	0.96226	1.93739	1.00000	1.00000
10	0.92646	1.87702	0.92645	1.87702	1.00001	1.00000
20	0.86027	1.76267	0.86027	1.76267	1.00000	1.00000
50	0.69876	1.46548	0.69876	1.46548	1.00000	1.00000
100	0.52012	1.09340	0.52013	1.09341	0.99998	0.99999
200	0.34989	0.65116	0.34990	0.65117	0.99997	0.99998
500	0.26256	0.26215	0.26256	0.26215	1.00000	1.00000
1000	0.26317	0.20302	0.26316	0.20302	1.00004	1.00000
2000	0.26365	0.20081	0.26365	0.20081	1.00000	1.00000
5000	0.26365	0.20081	0.26365	0.20081	1.00000	1.00000
10000	0.26365	0.20081	0.26365	0.20081	1.00000	1.00000

7 Check of Probability Distributions

In order to test the correct functioning of the sampling distributions, a test has been run with each type of distribution, in both standard and log-based form. This test case has been implemented and saved as *PDFs.cse*. A large number of samples (10000) have been used to get good statistics, note that the sampled parameters can be checked by checking the 'Do not calculate' box in the Calculate dialogue.

The mean and certain percentiles are evaluated and exported from AMBER using the statistical report and CDF plot functions.

7.1 Uniform

A uniform distribution in the range 1 to 3 is used. The min and max should be very close to the limits for 10000 samples (a few times 1E-4 typically). The mean and median should be very close to 2.0. The 25th and 75th percentiles should be close to 1.5 and 2.5.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	1.0001	1.0002
25%	1.5045	1.4999
50%	2.0113	1.9999
Mean	2.0000	2.0000
75%	2.4921	2.5000
Max	2.9999	3.0000

which all seem sensible.

The number of samples below 2.0 is 4941. For a binomial distribution we expect a deviation about the mean (5000) of $\pm 5000/\sqrt{10000}$, which is 50, so the observed deviation of 59 is entirely plausible.

In addition to the test above, the Latin Hypercube option was tested with the same uniform distribution but with only 100 samples. Figure 7.1-1 shows the frequency distribution generated by Monte Carlo sampling, whereas Figure 7.1-2 shows the result for Latin Hypercube sampling. The figures confirm the stratified sampling that is achieved with the Latin Hypercube approach.

Figure 7.1-1: Uniform Distribution, Monte Carlo Sampling

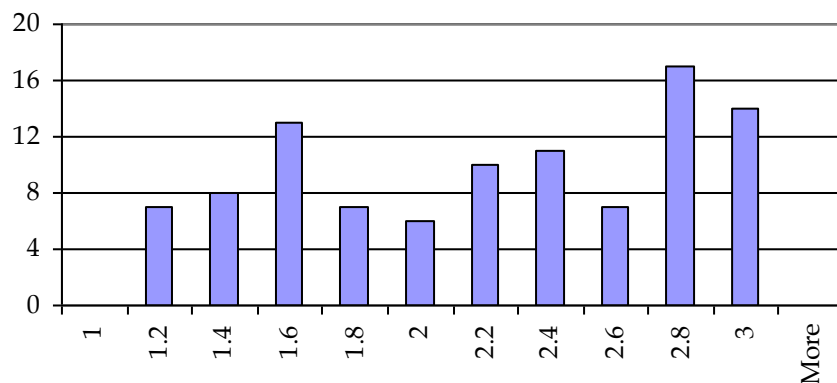
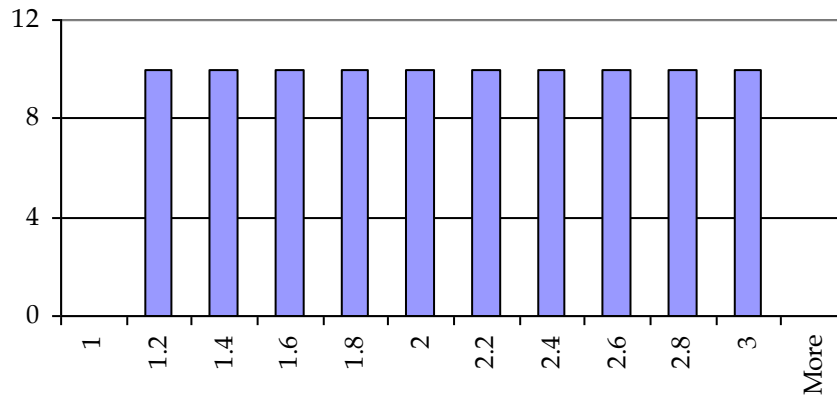


Figure 7.1-2: Uniform Distribution, Latin Hypercube Sampling



7.2 Log Uniform

A log-based uniform in the range 10^{-6} to 10^{-2} is used. The min and max should be close to the limits. The median should be close to 10^{-4} , while the 25th and 75th percentiles are close to 10^{-5} and 10^{-3} . The mean should be $(10^{-2}-10^{-6})/\ln(10^4)$, which is $1.0856 \cdot 10^{-3}$.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	1.0001E-6	1.0007E-6
25%	1.0491E-5	9.9965E-6
50%	9.7383E-5	9.9949E-5
Mean	1.0794E-3	1.0856E-3
75%	9.8118E-4	9.9908E-4
Max	9.9994E-3	9.9971E-3

which are all sensible.

The number of samples below 10^{-4} is 5047. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 47 is entirely plausible.

7.3 Gaussian

A full Gaussian has no upper and lower limits. We choose a mean of 10 and a standard deviation of 2. The min and max could be as many as 4 standard deviations from the mean (i.e. 2 and 18).

The mean and median should be close to 10. The 25th and 75th percentiles should be 8.651 and 11.349.

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The reported values are:

	Monte Carlo	Latin Hypercube
Min	2.9001	1.7104
25%	8.6482	8.6504
50%	10.0212	10.0000
Mean	10.0161	10.0000
75%	11.3773	11.3484
Max	17.7345	17.9078

which are all sensible.

The number of samples below 10 is 4953. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 47 is entirely plausible.

In addition to the test above, the Latin Hypercube option was tested with the same Gaussian distribution but with only 100 samples. Figure 7.3-1 shows the frequency distribution generated by Monte Carlo sampling, whereas Figure 7.3-2 shows the result for Latin Hypercube sampling. The figures confirm the stratified sampling that is achieved with the Latin Hypercube approach.

Figure 7.3-1: Gaussian Distribution, Monte Carlo Sampling

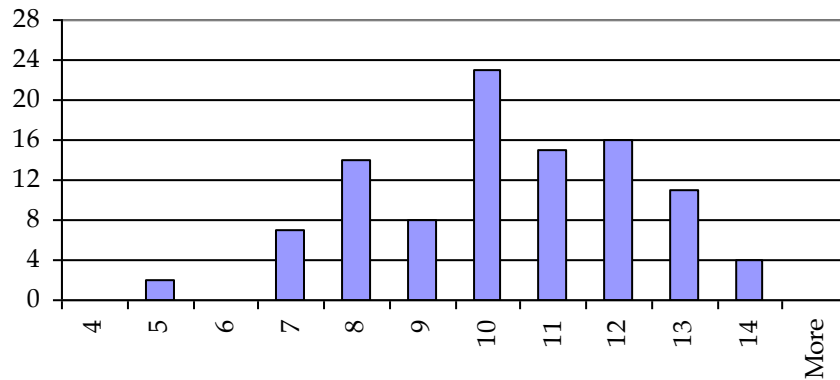
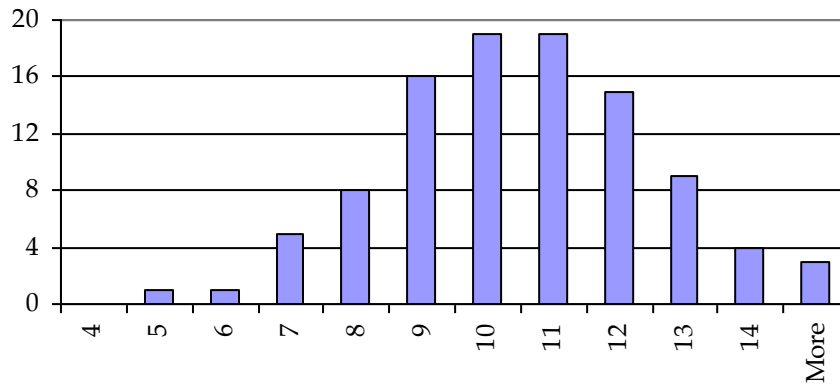


Figure 7.3-2: Gaussian Distribution, Latin Hypercube Sampling



7.4 Log Gaussian

For the Log Gaussian we choose a distribution with a log with mean 3 and standard deviation 1. The min should be around 0.1, the max 10^7 . The median should be 10^3 and the 25th and 75th percentiles should be 211.6 and 4726. Then mean should be $1.417E+4$.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	0.13431	0.11091
25%	202.51	211.46
50%	983.36	999.84
Mean	$1.2347E+4$	$1.3805E+4$
75%	4835.2	4724.7
Max	$1.9748E+6$	$7.8770E+6$

which are all sensible.

The number of samples below 1000 is 5024. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 24 is entirely plausible.

7.5 Truncated Gaussian

A truncated Gaussian has upper and lower limits. We choose the same mean and standard deviation as the Gaussian test (10 and 2), but with a range of 8 to 16 (i.e. 1 standard deviation below and 3 above).

The statistics for this are hard to calculate. Min and max will be near to 8 and 16. The 25th; 50th and 75th percentiles are 9.329, 10.397 and 11.603. The mean is 10.566.

AMBER 5.4 Verification Summary

The reported values are:

	Monte Carlo	Latin Hypercube
Min	8.0000	8.0006
25%	9.3327	9.3290
50%	10.4065	10.3966
Mean	10.5612	10.5656
75%	11.5995	11.6033
Max	15.9799	15.9871

which are all sensible.

The number of samples below the median (10.397) is 4977. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 23 is entirely plausible.

7.6 Triangular

The triangular distribution has a minimum, a peak, and a maximum. For the test, we choose 11, 14 and 15. This has the 75th percentile at 14, the 25th and median at 12.7321 and 13.4495. The mean is 13.3333.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	11.0429	11.0047
25%	12.7079	12.7319
50%	13.4377	13.4494
Mean	13.3255	13.3333
75%	14.0166	13.9998
Max	14.9861	14.9861

which are all sensible.

The number of samples below the median (13.4495) is 5038. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 38 is entirely plausible.

In addition to the test above, the Latin Hypercube option was tested with the same triangular distribution but with only 100 samples. Figure 7.3-1 shows the frequency distribution generated by Monte Carlo sampling, whereas Figure 7.3-2 shows the result for Latin Hypercube sampling. The figures confirm the stratified sampling that is achieved with the Latin Hypercube approach.

Figure 7.6-1: Triangular Distribution, Monte Carlo Sampling

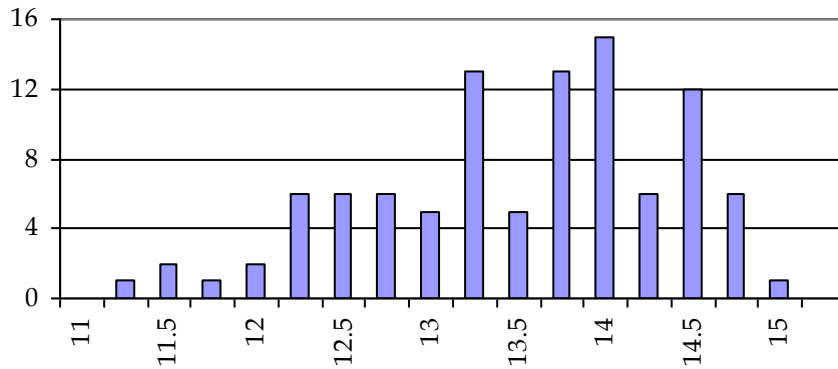
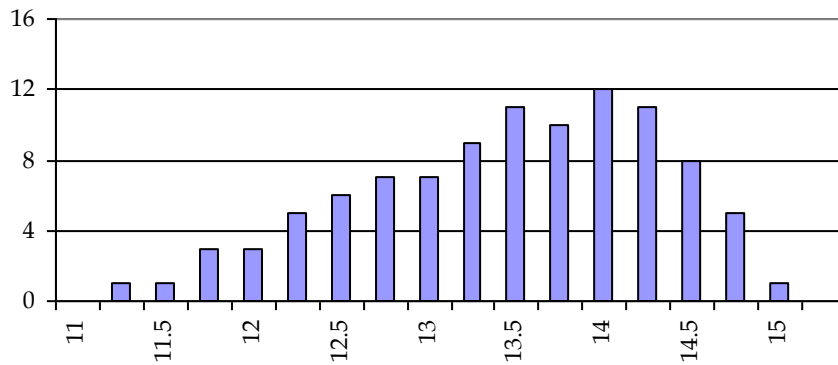


Figure 7.6-2: Triangular Distribution, Latin Hypercube Sampling



7.7 Log Triangular

The log triangular distribution has a minimum, a peak, and a maximum for the logarithm. For the test, we choose 1, 2 and 4, giving a range from 10 to 10^4 . The 25th, 50th and 75th percentiles are 73.46, 185.33 and 596.01. The mean is 611.10.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	10.071	10.030
25%	75.499	73.432
50%	188.79	185.33
Mean	621.21	611.12
75%	607.32	596.01
Max	9387.0	9715.8

which are all sensible.

The number of samples below the median (185.33) is 4956. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 44 is entirely plausible.

7.8 Beta

The beta distribution has a minimum, and a maximum with two parameters, A and B controlling the shape of the distribution. For the test, we choose a range -4 to -2 with A and B set to 0.5 and 1.5.

The 25th, 50th and 75th percentiles are -3.922, -3.674 and -3.194. The mean is -3.5.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	-4.0000	-4.0000
25%	-3.9214	-3.9219
50%	-3.6601	-3.6737
Mean	-3.4946	-3.5000
75%	-3.1839	-3.1945
Max	-2.0073	-2.0051

which are all sensible. The minimum being at -4 is because of the choice of A smaller than 1. This gives a singularity in the density at the end and thus generates values very close to the limit.

The number of samples below the median (-3.674) is 4905. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 95 is entirely plausible.

7.9 Log Beta

For the log beta test, we use the same parameters as the beta test, but for the log.

The 25th, 50th and 75th percentiles are 1.197E-4, 2.120E-4 and 6.393E-4. The mean is 7.32E-4.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	1.0000E-4	1.0000E-4
25%	1.1931E-4	1.1970E-4
50%	2.0787E-4	2.1200E-4
Mean	7.3186E-4	7.3225E-4
75%	6.3156E-4	6.3918E-4

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Max	9.8269E-3	9.8643E-3
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which are all sensible.

The number of samples below the median ($2.12E-4$) is 5072. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 72 is entirely plausible.

7.10 General CDF

The General CDF allows a piecewise linear CDF to be specified. This corresponds to a piecewise constant PDF (histogram). The test uses four equi-probable intervals, 1 to 2, 2 to 4, 4 to 7 and 7 to 8.

The 25th, 50th and 75th percentiles are at the interval boundaries: 2, 4 and 7. The mean is 4.375.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	1.0011	1.0004
25%	1.9857	1.9998
50%	4.0480	3.9998
Mean	4.3795	4.3750
75%	7.0029	6.9999
Max	8.0000	7.9999

which are all sensible.

The number of samples below the median (4) is 4955. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 45 is entirely plausible.

7.11 Log General CDF

For the Log General CDF we take the intervals (of the log) as -1 to 0, 0 to 1 and 1 to 1.6. We assign probabilities of 0.3, 0.5 and 0.2 to these.

The 25th, 50th and 75th percentiles are 0.6813, 2.5119 and 7.943. The min and max are 0.1 and 39.811. The mean is 6.3871.

The reported values are:

	Monte Carlo	Latin Hypercube
Min	0.1000	0.1000
25%	0.6598	0.6810
50%	2.4719	2.5116

AMBER 5.4 Verification Summary

Mean	6.4095	6.3871
75%	7.9123	7.9429
Max	39.7915	39.798

which are all sensible.

The number of samples below the median (2.5119) is 5038. As described above, for a binomial distribution we expect a deviation ± 50 , so the observed deviation of 38 is entirely plausible.

8 Correlation Checks

This section describes verification tests that demonstrate:

- ▲ That parameters are sampled independently; and
- ▲ That correlations can be specified.

8.1 Independent Sampling

To check that the separate sampled values are not correlated, two Gaussian distributions were generated, both with zero mean and unit variance and saved as *NoCorrelationCheck.cse*. The standard and rank correlation coefficients were generated in batch mode with a 10 000 sample Monte Carlo run:

Standard correlation coefficient: -0.0013473

Rank correlation coefficient: -0.00263604

Similarly, standard and rank correlation coefficients were generated in batch mode with a 10 000 sample Latin Hypercube run:

Standard correlation coefficient: -0.0072046

Rank correlation coefficient: -0.00443935

These results indicate a very low correlation, as expected.

8.2 Specifying Correlations

The ability to specify rank correlation coefficients has been tested by setting up a simple case with the parameters and correlations defined in Table 8.2-1. The specification therefore includes two separate correlation sets (Ppt, RunOff and Irrig forming one group and Kd and CF_Plant another), positive and negative correlations and different types of distribution.

Table 8.2-1: Definition of Parameters and Correlation Coefficients

Name	Distribution	Correlation
Ppt	Gaussian: mean = 0.98, SD = 0.095, minimum = 0	
RunOff	Gaussian: mean = 0.31, SD = 0.08, minimum = 0	To Ppt = 0.8
Irrig	Triangular: peak = 0.3, minimum = 0, maximum = 0.6	To Ppt = -0.9 To RunOff = -0.85
Kd	Lognormal: GM = 0.018, GSD = 10	
CF_Plant	0.03, GSD = 10	To Kd = -0.7

The case, *CorrelationCheck.cse*, was run with 10,000 samples. The resulting matrix of rank correlation coefficients is shown in Table 8.2-2 and proves a good match to those specified in Table 8.2-1. The table also provides confidence that no correlations are introduced between the separate parameter groups, with a maximum rank correlation coefficient of -0.0021, which is very low.

Table 8.2-2: Matrix of Rank Correlation Coefficients

Parameter	Ppt	Irrig	RunOff	Kd	CF_Plant
Ppt	1	-0.9057	0.8032	-1e-006	0.0001
Irrig	-0.9057	1	-0.8496	-0.0009	3e-005
RunOff	0.8032	-0.8496	1	-0.0021	0.0011
Kd	-1e-006	-0.0009	-0.0021	1	-0.6919
CF_Plant	0.0001	3e-005	0.0011	-0.6919	1

9 Pressure Tests

A further requirement of the AMBER 5.4 verification is pressure testing, in order to document the limits of the AMBER software in performing calculations and inform sensible application of the code. These tests look at the limits of transfer rates, number of compartments, number of contaminants and decays, user-entered large numbers, and at the issues of memory leakage and solver tolerance. The results are reported below.

The nature of pressure testing requires that large cases be used for some of the tests, some of these have been based on extensions of commercial cases and are therefore not available for distribution with the other verification cases. These cases are noted below.

9.1 Transfer Rates

A simple case, *PressureTest_TransferRate.cse*, was set up to investigate whether a maximum limit is encountered the rate of transfers. The case has two compartments and one transfer. The transfer is configured as non-depleting, as the large fluxes expected would soon empty a depleting compartment.

In this configuration, running the calculation with a transfer rates above $1\text{E}+154\text{ y}^{-1}$ using the Laplace solver caused the calculation to be halted and a series of error messages to appear. Up to and including this value, the calculations ran as expected. Such a rapid transfer is well beyond the bounds of sensible application.

When using the Time-Step solver, no problems were encountered before reaching the limit of large numbers (see below).

9.2 Compartments

The maximum number of compartments that AMBER can handle is largely a function of the computer system used and its available memory. Whilst it is difficult to identify a set limit of compartments, many models have been run comfortably with large numbers of compartments. For example, a recent commercial application includes 452 compartments and is run without any problems on a Microsoft Windows machine with 3GB of RAM. Also, a case with a single contaminant and a chain of over 1000 compartments operates as expected.

9.3 Contaminants and Decays

A recent commercial case file, developed for screening radionuclides, includes 1070 contaminants and 1160 decays. The case was extended to investigate whether limits are encountered for the number of contaminants and decays. The contaminants and decays were duplicated and the case run until errors were reported. No problems were encountered up to and including a case where 5350 contaminants and 5800 decays were used. This provides evidence that AMBER can handle a large number of contaminants and decays, well beyond the bounds of expected application.

9.4 Large Numbers

Using the simple case *PressureTest_TransferRate.cse*, described above, start amounts and transfer rates were increased to see how AMBER handles large numbers. Up to and including values of $1\text{E}+308$, the values were stored fine (regardless of units). However, above these values, the editor stored them as "1.#INF" (infinity). Even before calculations were run, the editor was unable to store larger numerical values; the program unsurprisingly prevents the results from being calculated and displays an error message when trying to use values of infinity. A similar process occurs in batch mode; when the file is re-saved the value of infinity replaces any numbers greater than $1\text{E}+308$. This is

because the software saves values to double-precision, and $1\text{E}+308$ is the maximum that can be stored in the allocated memory for this format – it is sufficiently large, however, to be unlikely to cause any problems.

9.5 Solver Tolerance

AMBER cases may involve simultaneous handling of both large and small numbers, differing by many orders of magnitude, in and between a system of compartments. The AMBER solvers, as with any numerical solvers, need to include a level of tolerance in relation to such situations.

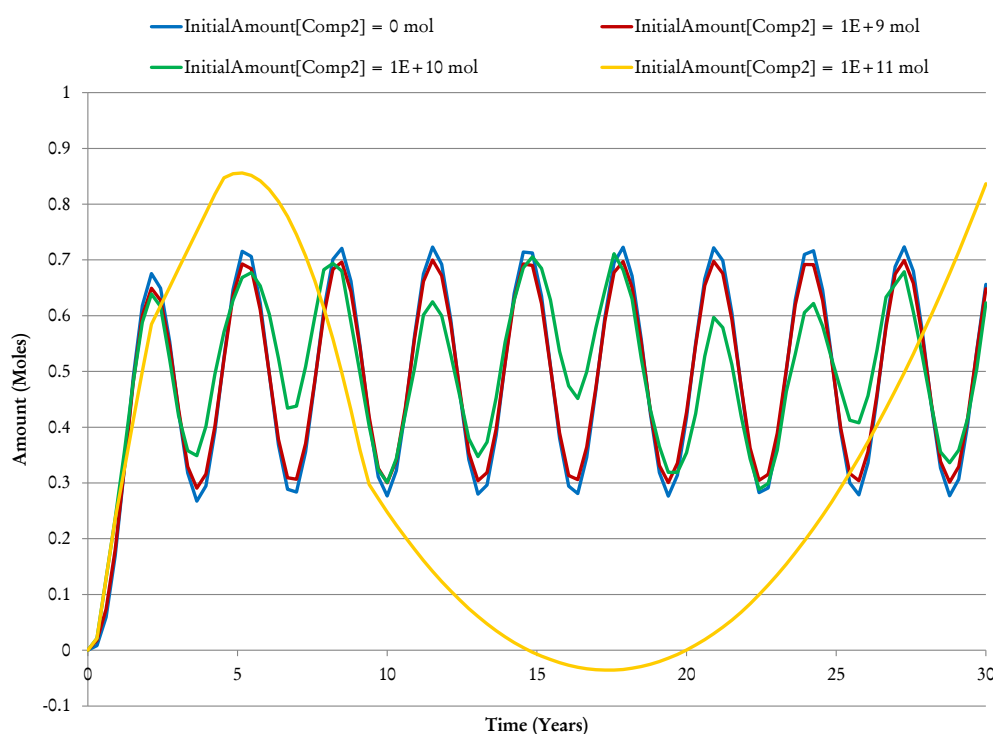
A test case, *PressureTest_SolverTolerance.cse* is set up to examine the practical implications of the AMBER solver tolerances, comprising of a single contaminant moving between two compartments with a transfer rate of 1 y^{-1} . There is a source flux of this contaminant into the first compartment at a rate equal to $\sin^2(t)\text{ mol y}^{-1}$, keeping the amount of contaminant in this compartment relatively constant, oscillating around $\sim 0.5\text{ mol}$. In the second compartment different start amounts are set, increasing from zero up to higher powers of ten. Monitoring the reported values in the first compartment then demonstrates the tolerance of the solver – as long as the values are reported as expected then the solver can handle the calculations, but if the values in the first compartment are not what is expected, then it can be seen that the solver cannot handle both the smaller fluxes into the first compartment and the large values held in the second compartment.

The calculations report values as expected up until the second compartment contains $1\text{E}+9$ moles of contaminant. Above this (i.e., when there were around 10 or more orders of magnitude between the largest and smallest values in the system), the reported values for the first compartment deviated significantly, as can be seen by the green line in Figure 9.5-1. For values of $1\text{E}+11$ mol and above (11 or more orders of magnitude between the largest and smallest values in the system), the model broke down and gave entirely incorrect results, as shown by the orange line in Figure 9.5-1.

This test case indicates that the accuracy of AMBER may begin to break down when evaluating amounts of contaminants that are more than ten orders of magnitude below the highest amounts in the system. Such solver tolerances are unavoidable and the results for AMBER are considered acceptable because such very small amounts are unlikely to be of interest in most applications. However, the results highlight the importance of exploring and questioning the results of any numerical code, including AMBER. Should such small results be related to observers of interest, then the modelling approach warrants further iteration, for example, by separating the part of the system where very small amounts are calculated into a separate AMBER model and importing fluxes from the source term.

It is emphasised that the solver tolerance is not a weakness in AMBER, but a practical issue that is relevant to any numerical solvers. Indeed, it is noted in Section 2 that AMBER performs very well in relation to other codes and even provides the benchmark against which other codes have been tested.

Figure 9.5-1: Solver Tolerance Test Results showing Calculated Amount in Compartment 1 with Deferring Initial Amounts in Compartment 2



10 AMBER 5.4 Tests

This section describes the testing that has been undertaken for the new features and development included in AMBER 5.4 (Section 10.1) and the tests that were undertaken to confirm that reported bugs have been fixed (Section 10.2). Test tests are listed in the order that the features are described in the AMBER 5.4 Release Note (Quintessa, 2010d). The simple nature of many of the tests means that there is no need to include specific test cases.

10.1 New Features and Developments in AMBER 5.4

- ▲ Icon and Appearance of the User Interface: The new icon is associated with the shortcuts, file association and is used within the user interface of the installed AMBER 5.4. The new icons/buttons used within the user interface have been checked and display correctly.
- ▲ Descriptions and Comments: AMBER 5.4 has been checked to verify that descriptions to be recorded against namesets, nameset selections, correlations and availability

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schemes. The inclusion of comments against specific parameter and mapping items has been checked and performs correctly.

- ▲ Reporting Defaults: The *Save Special* option to explicitly report the use of defaults in the text based case file has been checked, as has the loading of the special case file back via the user interface.
- ▲ Move to Q2DGrapher: AMBER 5.4 has been checked to ensure that QCharter is no longer available via the Graph Type dialog, that charting uses Q2DGrapher and that the Output to Excel functions correctly.
- ▲ Checking Observers and Availability before Calculation: AMBER 5.4 has been checked to ensure that errors in Observers and Availability Schemes are now identified prior to calculation.
- ▲ Show User Editable Decay Rates: AMBER 5.4 has been checked to ensure that decay rates are displayed in the Contams and Decays Tree when the User Editable DecayRate option is selected via the Decays window.
- ▲ Aligning Items via the Model Window: AMBER 5.4 has been checked to verify that selected Model window items can now be aligned via the context-sensitive menu that is accessed by right-clicking.
- ▲ Colour-Coding Arrows: AMBER 5.4 has been checked to ensure that arrows can be colour coded separately or all together via the *View | Colour | Arrows* menu.
- ▲ Displaying the List of Namesets Alphabetically: The NameSet window has been checked in AMBER 5.4 to ensure that NameSets can be listed alphabetically or in the order added to the case file.

10.2 Bug Fixes Implemented in AMBER 5.4

- ▲ Use of Namesets in Nameset Option Parameters: AMBER 5.4 has been checked to ensure that the NameSets used solely in NameSet Option parameters are not identified as being unused in the NameSet Window.
 - ▲ Nameset Option Crash: AMBER has been checked to ensure that it does not crash if a NameSet Option parameter is indexed over a NameSet that does not exist.
 - ▲ Navigator Freezing: AMBER 5.4 has been checked to verify that the submodel navigator no longer freezes when a particular combination of actions is undertaken.
 - ▲ Overlaps Following Alignment: AMBER 5.4 has been checked to confirm that a warning message is presented with a cancel option is the user tries to align Model Window items in a way that would result in overlaps.
-

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- ▲ **Checking Expressions Display:** AMBER 5.4 has been checked to ensure that re-checking expressions via the Expression Editor no longer results in a misleading expression breakdown in the Check tab.
- ▲ **Zero result at Final Output Time:** Cases that resulted in zero amounts at the final Result Time has been checked in AMBER 5.4 to verify that the behaviour no longer occurs.
- ▲ **Deleting Sub-Models:** AMBER 5.4 has been checked to ensure that information associated with nested submodels is correctly removed from the case file when submodels are deleted.
- ▲ **Auto-name Transfer Preference:** AMBER 5.4 has been checked to ensure that the user preference for auto-naming transfers is now correctly recalled.

11 Conclusions

The wide-ranging set of test cases documented here verify the correct functioning of AMBER in both deterministic and probabilistic modes.

These, together with the continuous testing that AMBER undergoes when it is applied to new cases, show that the code works well over a wide range of problem types.

Of course, no testing can rule out the possibility of there being undiscovered errors in the code. To help find these, all users should report any incorrect, or suspicious, behaviour so that it can be investigated and, if necessary, corrected in subsequent versions.

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