AMBER 6.8 Verification and Validation Summary

Quintessa Limited

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Quintessa

Summary

AMBER is a compartment modelling software tool developed by Quintessa Ltd.

This is the Verification and Validation Summary for the AMBER 6.8 software. AMBER 6.8 is a flexible software tool that allows the user to build their own dynamic compartment models to represent the migration and fate of contaminants in a system.

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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 (2025a and b).

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 validation of the models themselves, as opposed to the computer code, is the responsibility of the model developer who uses AMBER. A list of publications describing application of AMBER to various assessments, including those involving the development of models for application to experimental data, are given in the AMBER User Guide (Quintessa, 2025b).

However, in the process of validating 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 code intercomparisons are discussed in Section 2. Some published applications of AMBER involving the validation of the modelling of observational data are given in Section 3.

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 standard set of these tests and reports on their application to AMBER 6.8. These tests have been carried out for both the Windows and Linux versions of AMBER 6.8. The tests described in this report focus on checking that the correct solution is calculated by AMBER. This report is accompanied by electronic versions of the AMBER case files, which are referred to in the documentation of each test and are installed with the software.

The tests described here are as follows.

- Some simple cases with known solutions that have been used throughout AMBER's development are described in Section 4.
- A simple biosphere model, which checks the deterministic and probabilistic functioning of AMBER against documented results from a Nuclear Energy Agency (NEA) study, are described in Section 5.
- A comparison with a solubility-limited source term model, developed by AEA Technology for Nirex, is described in Section 6.
- A comparison with analytical and spreadsheet calculations for cases involving Langmuir Availability schemes are given in Section 7.
- A case using all the probability distributions available in AMBER to check that sensible values are generated is described in Section 8.
- Section 9 describes the results of cases used to test that sampling is properly random and that correlations are appropriately generated when specified.
- Section 10 summarises some tests that check the correct calculation of spatial properties in AMBER.

In this Verification and Validation Summary report, the performance of AMBER is evaluated by consideration of the reporting of outputs to several significant figures, the nature of which is described for each test. AMBER performs well for all these tests, giving confidence in the correct functioning of the code.

In addition, Section 11 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 12 summarises additional targetted tests for AMBER 6.8.

Brief conclusions are presented in Section 13, whilst references are provided in Section 14.

Verification of the outputs calculated with AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7, are presented in Appendix A.

2 Published Code Comparisons

AMBER has been applied in many projects. The AMBER User Guide (Quintessa, 2025b) 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 implementing similar models or the same equations.

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.

AMBER has since been used by SSM as part of their review of SKB's calculations for the KBS-3 repository for spent fuel, considering both near-field processes and radionuclide transport (Penfold, 2014) and landscape modelling and dose assessment calculations (Walke, 2014; Walke and Limer, 2014; Walke et al., 2015). AMBER has been used by SSM as part of their review of SKB's SR-PSU assessment of the long-term safety for the expansion of the final repository for low and intermediate level waste at Forsmark (Klos et al., 2017; Towler et al., 2017; Walke et al., 2017a, b). Most recently, SSM used AMBER to support their review of SKB's safety evaluation for a long-lived low and intermediate level radioactive waste disposal facility, SE-SFL (Geier et al., 2021). STUK used AMBER in their review of Posiva's TURVA-12 assessment for the spent fuel geological disposal facility at Olkiluoto, with a focus on radionuclide transport modelling (Towler et al., 2014). These reviews consisted a test of both the conceptual modelling approaches adopted by the waste management organisations, SKB and Posiva, and a test of their calculations against independent calculations undertaken using AMBER.

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 agreed with those obtained using other internationally recognised codes.

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 ERB2A 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 BIOMOVS II. QuantiSci (UK) developed an AMBER model for the C-14 release to a lake scenario (BIOMOVS, 1996a), whilst Ciemat (Spain) developed models for the Complementary Studies (BIOMOVS, 1996b) and lysimeter (BIOMOVS, 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 IRSN 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 Published Applications to Observational Data

AMBER has been applied in many projects. The AMBER User Guide (Quintessa, 2025b) 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 against observational data. In a number of these publications other software tools will have been validated against the same observational data.

In the 1990s, the BIOMOVS II programme sought to validate mathematical models for C-14 migration in both lakes and vegetated soils using observational data (BIOMOVS II 1996a, 1996c; Bird et al., 1999). AMBER was then used to look again at the modelling of the observational lake data by SSM in 2014 (Limer and Klos, 2014).

In the UK, the Food Standards Agency (FSA) requires a modelling capability for the transport of contaminants in terrestrial food chains in order to assess potential impacts of routine or accidental releases of contaminants to the atmosphere on food quality (Walke et al., 2021). The PRISM software uses a 'wrapped' version of food chain models implemented in the AMBER compartment modelling software with a bespoke Graphical User Interface (GUI) and direct access to a Microsoft Access database of parameter values to produce an integrated package capable of undertaking probabilistic assessments. It comprises of a Soil-Plant and an Animal model for trace contaminants (radionuclides and heavy metals) and the 'special' radionuclides C-14 and H-3. The Soil-Plant and Animal models were validated against published data sets during their development (Thorne et al., 2006; Walke, 2012).

In Sweden, the Swedish Radiation Safety Authority (SSM) have developed a model of the behaviour of C-14 in soils, vegetation and the atmosphere, SSPAM^{14}C, which has been applied to observational data collected by IRSN, both as part of a bi-lateral study (Limer et al., 2015), and a wider international BIOPROTA project (Limer et al., 2017).

In the Republic of Korea, KAERI developed a compartment model for the behaviour of tritium around the Wolsong nuclear power plants, comparing measured tritium concentrations in the top soil and deep soil water with model outputs (Choi et al., 2004).

In June 2022, the University of Ottawa published a PhD thesis entitled "An Assessment of Iodine-129 and Iodine-127 in Human Biological Materials with Modelling of Dietary Iodine Intake and Excretion" (Awwadh AlMarshadi, 2022). This thesis was concerned with iodine status and sources in human body, and measurements in human materials in the Canadian population. Using I-129 as a tracer, a new method was developed to extract I-129 from urine, and an existing method to extract I-129 from breastmilk refined. Subsequently, a biokinetic model of iodine, developed by Leggett (2017), was implemented in the AMBER compartment modelling software. This model was used to investigate the main sources of I-127 and I-129 in the Canadian diet based on daily food consumption survey data, and modelling of the urinary iodine concentration for adults and infants.

4 Simple Test Cases

The verification of AMBER 6.8 against three simple test cases is presented in this section. The purpose of these test cases is to verify the basic functionality of AMBER. All cases were run with default solver precision settings, which are as follows: Laplace solver, with a maximum order of 5. All AMBER results are presented rounded to six significant figures.

The verification of the outputs calculated by AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7 are presented in Appendix A, Appendix A.1.

4.1 SN2

This case is a simple system with three compartments and two contaminants (see Figure 1), which has been implemented in AMBER as *SN2.cse*. The transfer rates are piecewise constant.

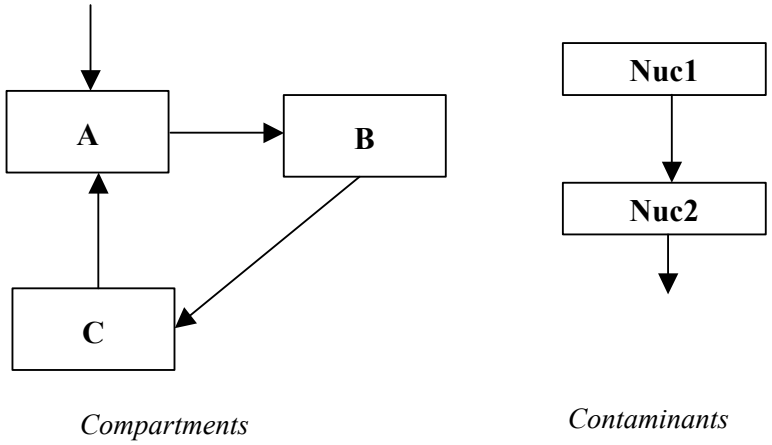

Figure 1. Structure of SN2

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. The initial transfer rates are given in Table 1. After 40 years they all fall by a factor of 100.

Table 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 (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.

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

The 10- and 100-year results are quoted as representative in Table 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 2. Comparison of SN2 Results with SPADE (moles)

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

4.2 SN5

SN5 tests a simple case with non-depleting transfers and local decay rates; the structure is illustrated in Figure 2.

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:

$$A = \mathrm{e}^{-\lambda t} \tag{4.1}$$

$$B = \frac{1-\mathrm{e}^{-\lambda t}}{\lambda} \tag{4.2}$$

$$C = \frac{t}{\lambda} - \frac{1-\mathrm{e}^{-\lambda t}}{\lambda^2} \tag{4.3}$$

where λ is the decay rate (y^{-1}).

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. The agreement is very good throughout.

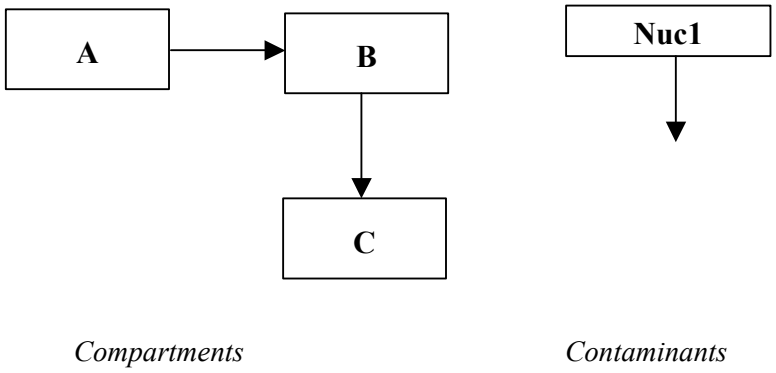

Figure 2. Structure of SN5

Table 3. Results of SN5 (moles), given to six significant figures

Time (y)	Compart-ment	Analytic	AMBER (Windows)		AMBER (Linux)	
			Laplace Solver	Time-step Solver	Laplace Solver	Time-step Solver
0.01	A	0.999900	0.999900	0.999900	0.999900	0.999900
0.01	B	0.00999950	0.00999950	0.00999**49**	0.00999950	0.00999**49**
0.01	C	4.99983E-5	4.99983E-5	**5.05133**E-5	4.99983E-5	**5.05133**E-5
10	A	0.904837	0.904837	0.904837	0.904837	0.904837
10	B	9.51626	9.51626	9.51626	9.51626	9.51626
10	C	48.3742	48.3742	48.3742	48.3742	48.3742
100	A	0.367879	0.367879	0.36787**2**	0.367879	0.36787**2**
100	B	63.2121	63.2121	63.212**8**	63.2121	63.212**8**
100	C	3678.79	3678.79	3678.7**2**	3678.79	3678.7**2**
1000	A	4.53999E-5	4.53999E-5	4.**61771**E-5	4.53999E-5	4.**61771**E-5
1000	B	99.9955	99.9955	99.995**4**	99.9955	99.995**4**
1000	C	90000.5	90000.5	90000.5	90000.5	90000.5

4.3 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).

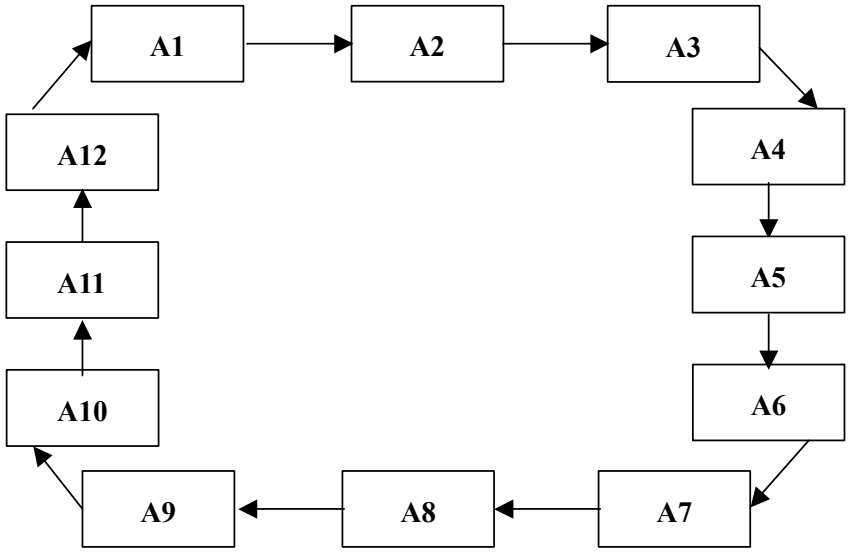

Figure 3. Structure of SN7

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:

$$\frac{\mathrm{d}A_n}{\mathrm{d}t} = \mu A_n - \mu A_{n-1} \tag{4.4}$$

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

$$A_n(t) = E_n \mathrm{e}^{-\gamma t} \tag{4.5}$$

from the governing equation it is clear that:

$$E_n = \frac{\mu}{\mu - \gamma} E_{n-1} \tag{4.6}$$

and the loop symmetry gives:

$$\left(\frac{\mu}{\mu - \gamma}\right)^N = 1. \tag{4.7}$$

The eigen-values are therefore given by:

$$\gamma^{(k)} = \mu \left(1 - \mathrm{e}^{-2\pi i k/N}\right) \tag{4.8}$$

with corresponding eigen-solutions:

$$E_n^{(k)} = \mathrm{e}^{2\pi i k n/N}. \tag{4.9}$$

This then leads to the solution:

$$A_n(t) = \sum_{k=1}^{N} \alpha^{(k)} E_n^{(k)} \mathrm{e}^{-\gamma^{(k)} t}, \tag{4.10}$$

where:

$$\alpha^{(k)} = \frac{1}{N} \sum_{n=1}^{N} A_n(0) E_n^{(k)} \tag{4.11}$$

From this, results at 20, 40, 60, 80 and 100 years have been calculated. These are presented in Table 4. Results are reported to six significant figures.

The test case is implemented in AMBER in *SN7.cse* and the results, using the time-step solver, are shown in Table 5. The digits that disagree are highlighted. The agreement is generally to 3-4 significant figures.

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 6. These results are very similar to those presented in Table 5, with only small differences at the sixth significant figure.

Table 4. Analytical Results for SN7

Compartment	Amounts (moles)				
	$t = 20$ y	$t = 40$ y	$t = 60$ y	$t = 80$ y	$t = 100$ y
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

Table 5. AMBER Results for SN7 [Identical for Windows and Linux OS]

Compartment	Amounts (moles)				
	$t = 20$ y	$t = 40$ y	$t = 60$ y	$t = 80$ y	$t = 100$ y
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

Table 6. AMBER Results for SN7 with a Faster Transfer Rate Added [Identical for Windows and Linux OS]

Compartment	Amounts (moles)				
	$t = 20$ y	$t = 40$ y	$t = 60$ y	$t = 80$ y	$t = 100$ y
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

5 Simple Biosphere Model

In the 1990s, the OECD Nuclear Energy Agency (NEA) Probabilistic Safety Assessment Group (PSAG) undertook an international code intercomparison exercise. One of the models included in that study was the PSACOIN Level 1B model, which is a biosphere model with multiple transfers, compartments and contaminants (NEA, 1993). Transfer rates are specified as formulae, and both deterministic and probabilistic results were calculated during that study.

As a validation of AMBER 6.8, the PSACOIN Level 1B model as described in NEA (1993) has been implemented in AMBER (*Level1B.cse*) and compared against results presented in that report.

The verification of the outputs calculated by AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7, are presented in Appendix A, Appendix A.2.

5.1 Deterministic

Initially, a precise match of transfer rates and model outputs 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 transfer rates quoted in Table B5 of NEA (1993) are matched within the AMBER implementation of the model (results not shown here).

Table D1 of NEA (1993) gives the Bq inventories in each compartment at several times. The outputs from the participants generally agree. In the AMBER case file implemented (*Level1B.cse*) the deterministic results are generated by calculating with the 'Best Estimates' sampling option selected in the Calculate dialogue. The model was implemented in AMBER with the base units of moles; to compare the inventories in each compartment in Bq the parameter M_comp is used. The AMBER results using the Laplace solver are compared against the AEAT results using MASCOT in Table 7, as this is a semi-analytic solution and should be the most accurate and can be directly compared. Results are presented to three significant figures.

The only significantly different result is for Pa-231 in Deep Soil at 1000 years; all the other amounts calculated by AMBER are well within 1% of those calculated by MASOT. Other participants give the result of 2.00E+6 Bq of Pa-231 in the Deep Soil at 1000 years, in agreement with AMBER, so it is supposed that the quoted result quoted for MASCOT is probably erroneous.

Given the good match seen with regards the calculated amount of contamination in different model compartments, the calculated dose results would be expected to match well also. A full set of calculated doses is given in Table D2 of NEA (1993). In Table 8 the U-235 decay chain for each pathway (D_Path[U_235]) results are compared in detail. Except for the external dose calculated at 1 year and the dose from ingesting milk and 100,000 years, the AMBER results are the same as the MASCOT results to two significant figures. However, the external dose rate calculated by AMBER after 1 year, and the dose from ingesting milk at 10,000 years, do agree with the values reported by other participants (as reported to two significant figures).

5.2 Stochastic

In comparing 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 (see Section 7.2.3 of the Reference Manual).

Table D3 of NEA (1993) gives the summary of the mean, standard deviation and Chebyshev 95% confidence limit for the calculated total dose for both C14 and the U-235 decay chain obtained by participants using Monte Carlo analysis. As can be seen in Table 9, the AMBER results for both C-14 and the U-235 decay chain agree well with the ranges reported by the PSACOIN Level 1B participants.

Table 7. Comparison of AMBER and Mascot Amounts (Bq) for Level1B; three significant figures

Time	Amount (Bq)								
	AMBER (Windows)			AMBER (Linux)			MASCOT		
	1	1000	100000	1	1000	100000	1	1000	100000
Nuclide	**Compartment: Water**								
C14	4.67E+3	2.71E+3	2.20E-3	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	3.42E+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	7.25E-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	6.19E+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	3.87E+3	3.14E-3	1.20E+3	3.86E+3	3.13E-3
U235	8.70E-1	1.08E+1	8.46E+0	8.70E-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	1.63E-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	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	1.80E+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	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	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	4.62E+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	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	1.63E+5	1.06E+8	1.13E+8
Pa231	3.45E+0	2.00E+6	6.81E+7	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	5.42E-2	2.00E+6	7.12E+7

Table 8. Comparison of AMBER and Mascot Dose Rates for Level1B from the U-235 Decay Chain reported to two significant figures

Time	Dose (Sv/y)								
	AMBER (Windows)			AMBER (Linux)			MASCOT		
	1	1000	100000	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	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	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	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	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	1.2E-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	1.9E-14	2.0E-9	2.3E-9
External	3.9E-14	4.1E-9	4.8E-9	3.9E-14	4.1E-9	4.8E-9	4.0E-14	4.2E-9	4.8E-9

Table 9. Mean Stochastic Results for Level1B – Windows installation

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

6 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 for releases from a repository into a geosphere (Robinson et al., 1988). The model calculates toxicity levels in the near field and effective leach rates from the near-field, using the time-step solver, for 55 nuclides, including stable species. The model has been implemented in AMBER as *R11854.cse*, which is the report reference number.[1]

For the purposes of verification, comparisons are made with:

- the maximum near-field toxicity (unitless) and Time of Occurrence (years) for each nuclide where the maximum toxicity is more than 0.1; and
- the initial and maximum effective leach rates (to 10^6 years) for each element.

For the maximum near-field toxicity (see Table 10), the peaks calculated by AMBER are typically within 1% of the values reported by Robinson et al. (1988), when reported to three significant figures. However, there are some exceptions: Pu-238, Pu-240, Pu-242, Am-242m and Am-243. It is thought that these discrepancies could be caused by data errors in the original report or by numerical issues. None are serious enough to cause any concern.

With respect to the initial and maximum leach rates (see Table 11), the rates calculated by AMBER agree exactly with those reported in Robinson et al. (1988), as reported to two significant figures.

The verification of the outputs calculated by AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7, are presented in Appendix A, Appendix A.3.

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

Table 10. Comparison of AMBER Maximum Toxicity (-) with R11854

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

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

Table 11. Comparison of AMBER Leach Rates with R11854 (y^{-1})

Element	AMBER (Windows)		AMBER (Linux)		R11854	
	Initial Leach Rate	Maximum Leach Rate	Initial Leach Rate	Maximum Leach Rate	Initial Leach Rate	Maximum Leach Rate
H	8.0E-3	8.0E-3	8.0E-3	8.0E-3	Not given	Not given
C	8.1E-4	7.7E-3	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	8.2E-9	8.3E-9
Se	7.7E-3	7.7E-3	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	1.6E-3	1.6E-3
Zr	1.3E-7	1.5E-7	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	7.7E-3	7.7E-3
Tc	1.5E-5	2.0E-4	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	7.7E-3	7.7E-3
I	7.7E-3	7.7E-3	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	1.6E-3	1.6E-3
Sm	2.7E-9	2.7E-9	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	7.7E-3	7.7E-3
Ra	1.6E-3	1.6E-3	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	2.0E-4	2.0E-4
Th	2.0E-6	2.0E-6	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	2.0E-4	2.0E-4
U	2.3E-13	2.3E-13	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	2.0E-6	2.0E-6
Pu	7.5E-9	2.0E-6	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	4.5E-7	2.0E-6
Cm	2.0E-6	2.0E-6	2.0E-6	2.0E-6	2.0E-6	2.0E-6

7 Langmuir Availability

To test the correct functioning of the Langmuir Availability scheme within AMBER, two scenarios have been considered. In the first scenario, a simple limiting case with a single contaminant and single source is modelled and compared with an analytic result. In the second scenario, a shared availability scheme with a separately coded solution (using a larger number of simple timesteps) is considered.

The verification of the outputs calculated by AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7, are presented in Appendix A, Appendix A.4.

7.1 Simple Limiting Case

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

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\lambda A + s - \mu A \frac{A+\alpha}{A+\beta}. \tag{7.1}$$

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

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -(\lambda+\mu)A + s - \mu\alpha. \tag{7.2}$$

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

$$A = A_0 \mathrm{e}^{-(\lambda+\mu)t}, \tag{7.3}$$

where A_0 is the initial amount (moles).

Here $A_0 = 1$ (moles), $\lambda = 0.001$ (y^{-1}), $\mu = 0.01$ (y^{-1}), $\alpha = 0.5$ (moles) and $\beta = 10^{-20}$ (moles). 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 using the time-step solver can be directly compared with the analytical solution (see Table 12); results are reported to four significant figures. As can be seen, the match is very good throughout.

7.2 Shared Langmuir Case

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

$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\lambda_A A + s_A - \mu_A A \frac{A+B+\alpha}{A+B+\beta}, \tag{7.4}$$

$$\frac{\mathrm{d}B}{\mathrm{d}t} = -\lambda_A A - \lambda_B B + s_B - \mu_B B \frac{A+B+\alpha}{A+B+\beta}. \tag{7.5}$$

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.

This test case is implemented in *SharedLangmuirCase.cse* and the results using the time-step solver can be directly compared with the analytical solution (see Table 13). The agreement obtained is excellent, confirming the correct behaviour of the Langmuir calculation.

Table 12. AMBER and Analytical Results for Simple Langmuir Solutions (moles); four significant figures

Time	AMBER (Windows)	AMBER (Linux)	Analytic	Ratio
0	1.000E+0	1.000E+0	1.000E+0	1.000
1	9.891E-1	9.891E-1	9.891E-1	1.000
2	9.782E-1	9.782E-1	9.782E-1	1.000
5	9.465E-1	9.465E-1	9.465E-1	1.000
10	8.958E-1	8.958E-1	8.958E-1	1.000
20	8.025E-1	8.025E-1	8.025E-1	1.000
50	5.7**70**E-1	5.7**70**E-1	5.769E-1	1.000
100	3.329E-1	3.329E-1	3.329E-1	1.000
200	1.108E-1	1.108E-1	1.108E-1	1.000
500	4.08**6**E-3	4.08**6**E-3	4.087E-3	1.000
1000	1.6**69**E-5	1.6**69**E-5	1.670E-5	0.999
1200	1.8**49**E-6	1.8**49**E-6	1.850E-6	0.999
1500	6.8**08**E-8	6.8**08**E-8	6.830E-8	0.997
2000	2.7**61**E-10	2.7**61**E-10	2.790E-10	0.990

Table 13. AMBER and Analytical Results for Shared Langmuir Schemes (moles)

Time	AMBER (Windows)		AMBER (Linux)		Spreadsheet		Ratio (Analytic/Linux)	
	A	B	A	B	A	B	A	B
0	1.00000	2.00000	1.00000	2.00000	1.00000	2.00000	1.00000	1.00000
1	0.99229	1.98730	0.99229	1.98730	0.99229	1.98730	1.00000	1.00000
2	0.98466	1.97468	0.98466	1.97468	0.98466	1.97468	1.00000	1.00000
5	0.96226	1.93739	0.96226	1.93739	0.96226	1.93739	1.00000	1.00000
10	0.9264**6**	1.87702	0.9264**6**	1.87702	0.92645	1.87702	1.00001	1.00000
20	0.86027	1.76267	0.86027	1.76267	0.86027	1.76267	1.00000	1.00000
50	0.69876	1.46548	0.69876	1.46548	0.69876	1.46548	1.00000	1.00000
100	0.5201**2**	1.0934**0**	0.5201**2**	1.0934**0**	0.52013	1.09341	0.99998	0.99999
200	0.349**89**	0.6511**6**	0.349**89**	0.6511**6**	0.34990	0.65117	0.99997	0.99998
500	0.26256	0.26215	0.26256	0.26215	0.26256	0.26215	1.00000	1.00000
1000	0.2631**7**	0.20302	0.2631**7**	0.20302	0.26316	0.20302	1.00004	1.00000
2000	0.26365	0.20081	0.26365	0.20081	0.26365	0.20081	1.00000	1.00000
5000	0.26365	0.20081	0.26365	0.20081	0.26365	0.20081	1.00000	1.00000
10000	0.26365	0.20081	0.26365	0.20081	0.26365	0.20081	1.00000	1.00000

8 Check of Probability Distributions

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 (10,000 for both Monte Carlo and Latin Hypercube sampling methods) 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 (25th, 50th and 75th) are evaluated and exported from AMBER using the statistical report and CDF plot functions. These are compared against those expected from the properties of the distributions under consideration.

The verification of the outputs calculated by AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7, are presented in Appendix A, Appendix A.5.

8.1 Uniform Distribution

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 (the same when using either the Windows or Linux operating systems) are given in Table 14. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics are close to the values expected, agreeing if reported to two significant figures.

The number of samples below 2.0 is 4941 with full Monte Carlo sampling. For a binomial distribution we expect a deviation about the mean (5000) of $5000 \pm /\sqrt{10000}$, 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 4 shows the frequency distribution generated by Monte Carlo sampling, whereas Figure 5 shows the result for Latin Hypercube sampling. The figures confirm the stratified sampling that is achieved with the Latin Hypercube approach.

Table 14. Uniform Distribution Statistics (AMBER)

	Monte Carlo	**Latin Hypercube**
Min	1.0001	1.0002
25%	1.5046	1.5000
50%	2.0113	2.0000
Mean	2.0000	2.0000
75%	2.4922	2.5000
Max	2.9999	3.0000

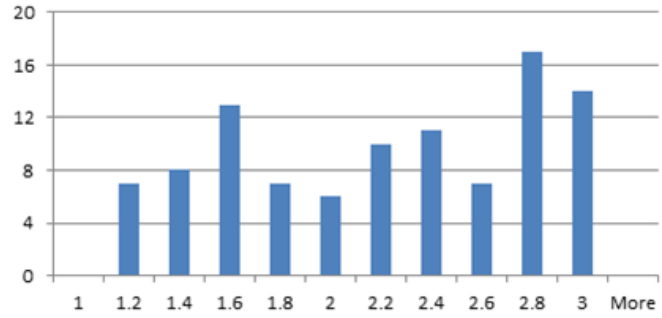

Figure 4. Uniform Distribution, Monte Carlo Sampling, 100 Samples

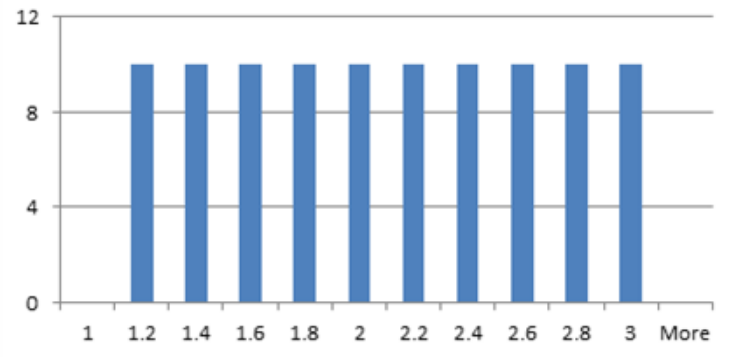

Figure 5. Uniform Distribution, Latin Hypercube Sampling, 100 Samples

8.2 Log Uniform Distribution

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 1.0856×10^{-3}.

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 15. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics generally lie close to the values expected, agreeing with them if reported to two significant figures.

The one exception is the median as calculated with the Monte Carlo sampling. The number of samples below 10^{-4} is 5047 with full Monte Carlo sampling. As described above, for a binomial distribution we expect a deviation ±50, so the observed deviation of 47 is entirely plausible.

Table 15. Log Uniform Distribution Statistics (AMBER)

	Monte Carlo	**Latin Hypercube**
Min	1.0001E-6	1.0007E-6
25%	1.0493E-5	1.0004E-5
50%	9.7388E-5	9.9990E-5
Mean	1.0794E-3	1.0856E-3
75%	9.8133E-4	9.9940E-4
Max	9.9994E-3	9.9971E-3

8.3 Gaussian Distribution

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.

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 16. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics lie very close to the values expected.

The number of samples below 10 is 4953 with full Monte Carlo sampling. 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 6 shows the frequency distribution generated by Monte Carlo sampling, whereas Figure 7 shows the result for Latin Hypercube sampling. The figures confirm the stratified sampling that is achieved with the Latin Hypercube approach.

Table 16. Gaussian Distribution Statistics (AMBER)

	Monte Carlo	Latin Hypercube
Min	2.9001	1.7104
25%	8.6511	8.6510
50%	10.0215	10.0001
Mean	10.0161	10.0000
75%	11.3774	11.3486
Max	17.7345	17.9078

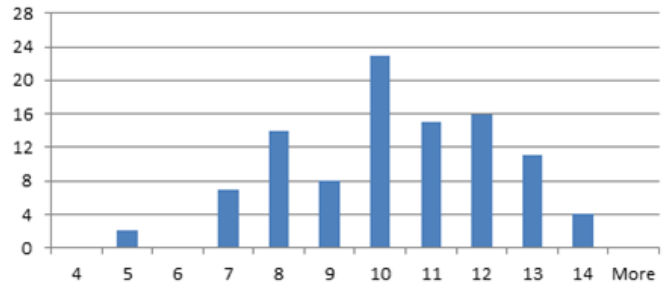

Figure 6. Gaussian Distribution, Monte Carlo Sampling, 100 Samples

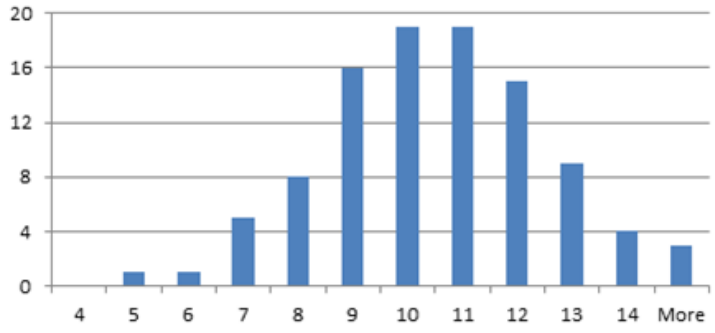

Figure 7. Gaussian Distribution, Latin Hypercube Sampling, 100 Samples

8.4 Log Gaussian Distribution

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. The mean should be 1.417E+4.

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 17. Except for the 25th and 75th percentiles obtained with the Latin Hypercube sampling and medians arising by either sampling method, the summary statistics do not lie as close to the values expected as with the previous distributions considered.

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

Table 17. Log Gaussian Distribution Statistics (AMBER)

	Monte Carlo	**Latin Hypercube**
Min	0.13431	0.11091
25%	202.55	211.59
50%	983.65	1000.1
Mean	1.2347E+4	1.3805E+4
75%	4838.3	4725.2
Max	1.9748E+6	7.8770E+6

8.5 Truncated Gaussian Distribution

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. The 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.

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 18. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics lie close to the values expected.

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

Table 18. Truncated Gaussian Distribution Statistics (AMBER)

	Monte Carlo	Latin Hypercube
Min	8.0000	8.0006
25%	9.3329	9.3292
50%	10.4068	10.3968
Mean	10.5612	10.5656
75%	11.5997	11.6034
Max	15.9799	15.9871

8.6 Triangular Distribution

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

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 19. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics lie close to the values expected.

The number of samples below the median (13.4495) is 5038 with full Monte Carlo sampling. 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 8 shows the frequency distribution generated by Monte Carlo sampling, whereas Figure 9 shows the result for Latin Hypercube sampling. The figures confirm the stratified sampling that is achieved with the Latin Hypercube approach.

Table 19. Triangular Distribution Statistics (AMBER)

	Monte Carlo	Latin Hypercube
Min	11.0429	11.0047
25%	12.7082	12.7322
50%	13.4380	13.4496
Mean	13.3255	13.3333
75%	14.0168	13.9999
Max	14.9861	14.9861

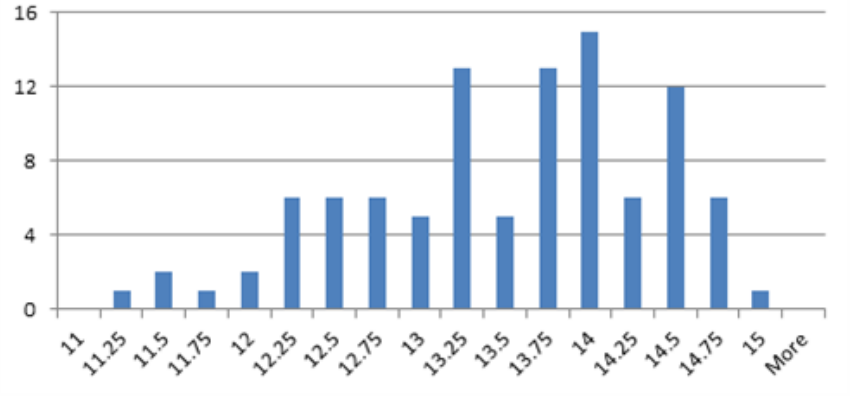

Figure 8. Triangular Distribution, Monte Carlo Sampling, 100 Samples

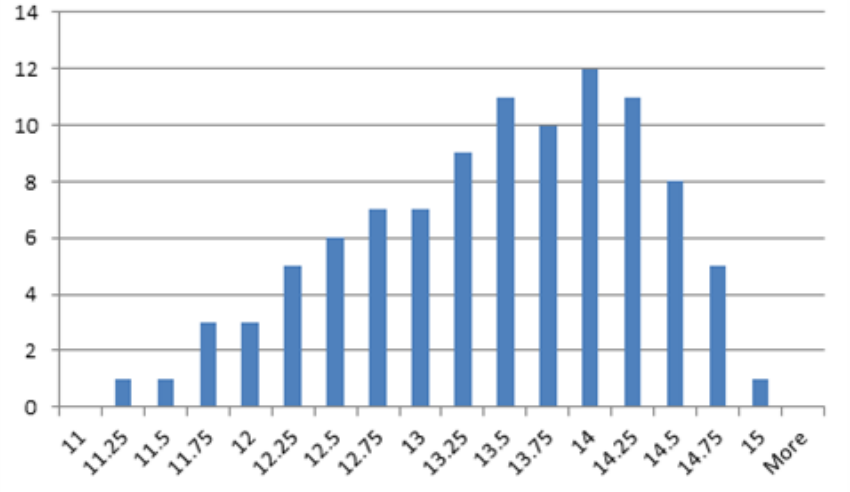

Figure 9. Triangular Distribution, Latin Hypercube Sampling, 100 Samples

8.7 Log Triangular Distribution

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 104. The 25th, 50th and 75th percentiles are 73.46, 185.33 and 596.01. The mean is 611.10.

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 20. Except for the 25th percentile for the Monte Carlo sampling, the summary statistics lie very close to the values expected for both sampling methods.

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

Table 20. Log Triangular Distribution Statistics (AMBER)

	Monte Carlo	**Latin Hypercube**
Min	10.071	10.030
25%	75.525	73.455
50%	188.81	185.34
Mean	621.21	611.12
75%	607.38	596.05
Max	9387.0	9715.8

8.8 Beta Distribution

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 (the same when using either the Windows or Linux operating systems) are given in Table 21. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics lie very close to the values expected.

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 with full Monte Carlo sampling. As described above, for a binomial distribution we expect a deviation ± 50, so the observed deviation of 95 is entirely plausible.

Table 21. Beta Distribution Statistics (AMBER)

	Monte Carlo	Latin Hypercube
Min	−4.0000	−4.0000
25%	−3.9214	−3.9218
50%	−3.6600	−3.6737
Mean	−3.4946	−3.5000
75%	−3.1839	−3.1944
Max	−2.0073	−2.0051

8.9 Log Beta Distribution

For the log beta test, we use the same parameters as the beta test, but for the log. The 25^{th}, 50^{th} and 75^{th} percentiles are 1.197E-4, 2.120E-4 and 6.393E-4. The mean is 7.32E-4.

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 22. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics lie very close to the values expected.

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

Table 22. Log Beta Distribution Statistics (AMBER)

	Monte Carlo	Latin Hypercube
Min	1.0000E-4	1.0000E-4
25%	1.1931E-4	1.1972E-4
50%	2.0787E-4	2.1202E-4
Mean	7.3186E-4	7.3225E-4
75%	6.3210E-4	6.3922E-4
Max	9.8269E-3	9.8643E-3

8.10 General CDF Distribution

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

The reported values (the same when using either the Windows or Linux operating systems) are given in Table 23. For both the Monte Carlo and Latin Hypercube sampling methods, the summary statistics lie very close to the values expected.

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

Table 23. General CDF Distribution Statistics (AMBER)

	Monte Carlo	**Latin Hypercube**
Min	1.0011	1.0004
25%	1.9858	2.0001
50%	4.0488	4.0004
Mean	4.3795	4.3750
75%	7.0030	7.0000
Max	8.0000	7.9999

8.11 Log General CDF Distribution

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 25^{th}, 50^{th} and 75^{th} 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 (the same when using either the Windows or Linux operating systems) are given in Table 24. Except for the 25^{th} percentile for the Monte Carlo sampling, the summary statistics lie very close to the values expected for both sampling methods.

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

Table 24. Log General CDF Distribution Statistics (AMBER)

	Monte Carlo	Latin Hypercube
Min	0.1000	0.1000
25%	0.6606	0.6814
50%	2.4730	2.5119
Mean	6.4095	6.3871
75%	7.9124	7.9437
Max	39.7915	39.7980

9 Correlation Checks

This section describes verification tests that demonstrate:

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

Verification that the behaviours reported below for AMBER 6.8 were also seen in previous versions of AMBER, in this instance AMBER 6.7, are given in Appendix A, Appendix A.6.

9.1 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 for each of the Monte Carlo and Latin Hypercube sampling methods (Table 25). These results indicate a very low correlation, as expected. The same results were recorded when using either the Windows or Linux operating systems.

Table 25. Standard and Ranked Correlation Coefficients in Independent Sampling Case

Statistic	Monte Carlo	Latin Hypercube
Standard correlation coefficient	-0.0013473	-0.0072046
Rank correlation coefficient	-0.00263604	-0.00443935

9.2 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 26. 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. The case, *CorrelationCheck.cse*, was run with 10,000 samples.

The resulting matrix of rank correlation coefficients is shown in Table 27 and proves a good match to those specified in Table 26. The table also provides confidence that no correlations are introduced between the separate parameter groups, with a maximum rank correlation coefficient of -0.0022, which is very low.

Table 26. 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

Table 27. Matrix of Rank Correlation Coefficients [Same for both Windows and Linux operating systems]

Parameter	Ppt	Irrig	RunOff	Kd	CF_Plant
Ppt	1	-0.9070	0.8075	-1e-005	-0.0013
Irrig	-0.9070	1	-0.8536	-0.0005	0.0014
RunOff	0.8075	-0.8536	1	-0.0022	-0.0005
Kd	-1e-005	-0.0005	-0.0022	1	-0.6913
CF_Plant	-0.0013	0.0014	-0.0005	-0.6913	1

10 Spatial Parameter Tests

Compartments can be assigned spatial dimensions from which AMBER is able to calculate a range of properties, including compartment volumes, interface areas and transfer distances. These spatial parameters are tested by comparison with analytical calculations of the same properties. From AMBER 6.3, floating point calculations of spatial parameters are undertaken to double precision, whereas prior releases undertook these calculations to single precision.

The verification of the outputs calculated by AMBER 6.8 versus previous releases of AMBER, in this instance AMBER 6.7, are presented in Appendix A, Appendix A.7.

10.1 ISAM Vault Test Case

The example case *Vault.cse* was used to test the methods used to determine the SpatialVolume, SpatialTransferArea, SpatialTransferDistance and SpatialTopArea parameters. Its geometry is shown in Figure 10.

The spatial parameters generated by AMBER for a representative sample of compartments are compared with analytical solutions in Table 28 to Table 31. Results are given to 5 decimal places; reported to this level the AMBER outputs agree exactly with the analytic solutions.

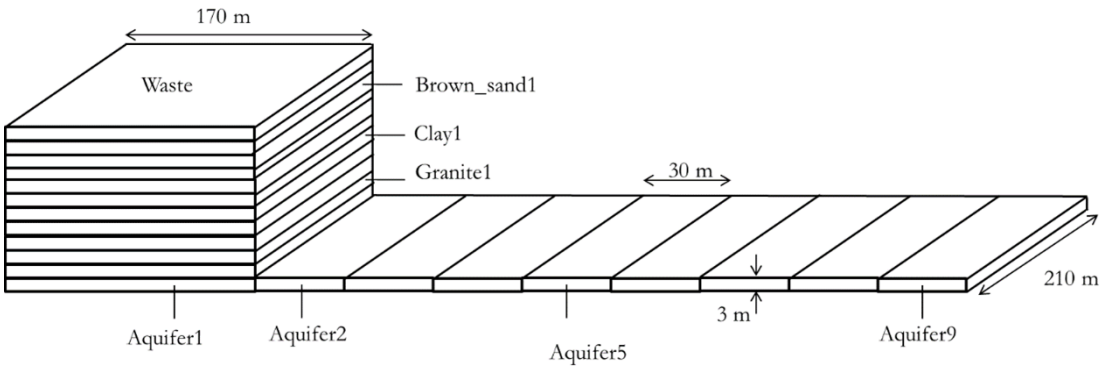

Figure 10. ISAM Vault test case geometry

Table 28. ISAM Vault: SpatialVolume parameter values (m^3)

Compartment	AMBER (Windows)	AMBER (Linux)	Analytic
Aquifer 1	1.07100E+5	1.07100E+5	1.07100E+5
Aquifer 2	1.89000E+4	1.89000E+4	1.89000E+4
Brown Sand 1	9.99600E+4	9.99600E+4	9.99600E+4
Brown Sand 3	1.03530E+5	1.03530E+5	1.03530E+5
Clay 1	9.63900E+4	9.63900E+4	9.63900E+4
Clay 3	9.28200E+4	9.28200E+4	9.28200E+4
Granite 1	1.16025E+5	1.16025E+5	1.16025E+5
Waste	3.21300E+5	3.21300E+5	3.21300E+5

Table 29. ISAM Vault: SpatialTransferArea parameter values (m^2)

Transfer	AMBER (Windows)	AMBER (Linux)	Analytic
Abstraction (Well – Sink)	0.00000E+0	0.00000E+0	0.00000E+0 (not spatial)
Disp_back 1 (Aquifer 1 – Aquifer 2)	6.30000E+2	6.30000E+2	6.30000E+2
Leaching (Waste – Concrete Base)	3.57000E+4	3.57000E+4	3.57000E+4

Table 30. ISAM Vault: SpatialTransferDistance parameter values (m)

Transfer	AMBER (Windows)	AMBER (Linux)	Analytic
Disp_back 1 (Aquifer 1 – Aquifer 2)	1.00000E+2	1.00000E+2	1.00000E+2
Disp_back2	3.00000E+1	3.00000E+1	3.00000E+1
Disp_back3	3.00000E+1	3.00000E+1	3.00000E+1
Disp_back4	3.00000E+1	3.00000E+1	3.00000E+1
Leaching (Waste – Concrete Base)	4.65000E+0	4.65000E+0	4.65000E+0
Unsat_flow1	1.50000E+0	1.50000E+0	1.50000E+0
Unsat_flow11	3.25000E+0	3.25000E+0	3.25000E+0
Unsat_flow19	3.15000E+0	3.15000E+0	3.15000E+0

Table 31. ISAM Vault: SpatialTopArea parameter values (m^2)

Compartment	AMBER (Windows)	AMBER (Linux)	Analytic
Aquifer 1	3.5700E+4	3.5700E+4	3.5700E+4
Aquifer 2	6.3000E+3	6.3000E+3	6.3000E+3
Brown Sand 1	3.5700E+4	3.5700E+4	3.5700E+4
Brown Sand 3	3.5700E+4	3.5700E+4	3.5700E+4
Clay 1	3.5700E+4	3.5700E+4	3.5700E+4
Clay 3	3.5700E+4	3.5700E+4	3.5700E+4
Granite 1	3.5700E+4	3.5700E+4	3.5700E+4
Waste	3.5700E+4	3.5700E+4	3.5700E+4

10.2 Non-Cuboid Geometry

For this test, the spatial parameters were calculated for a simple spatial model with non-cuboid geometry, shown in Figure 11. This test case is also implemented in *SpatialParameters.cse*.

The results from this model are compared with analytical solutions in Table 32 to Table 35. There is good agreement within 5 significant figures.

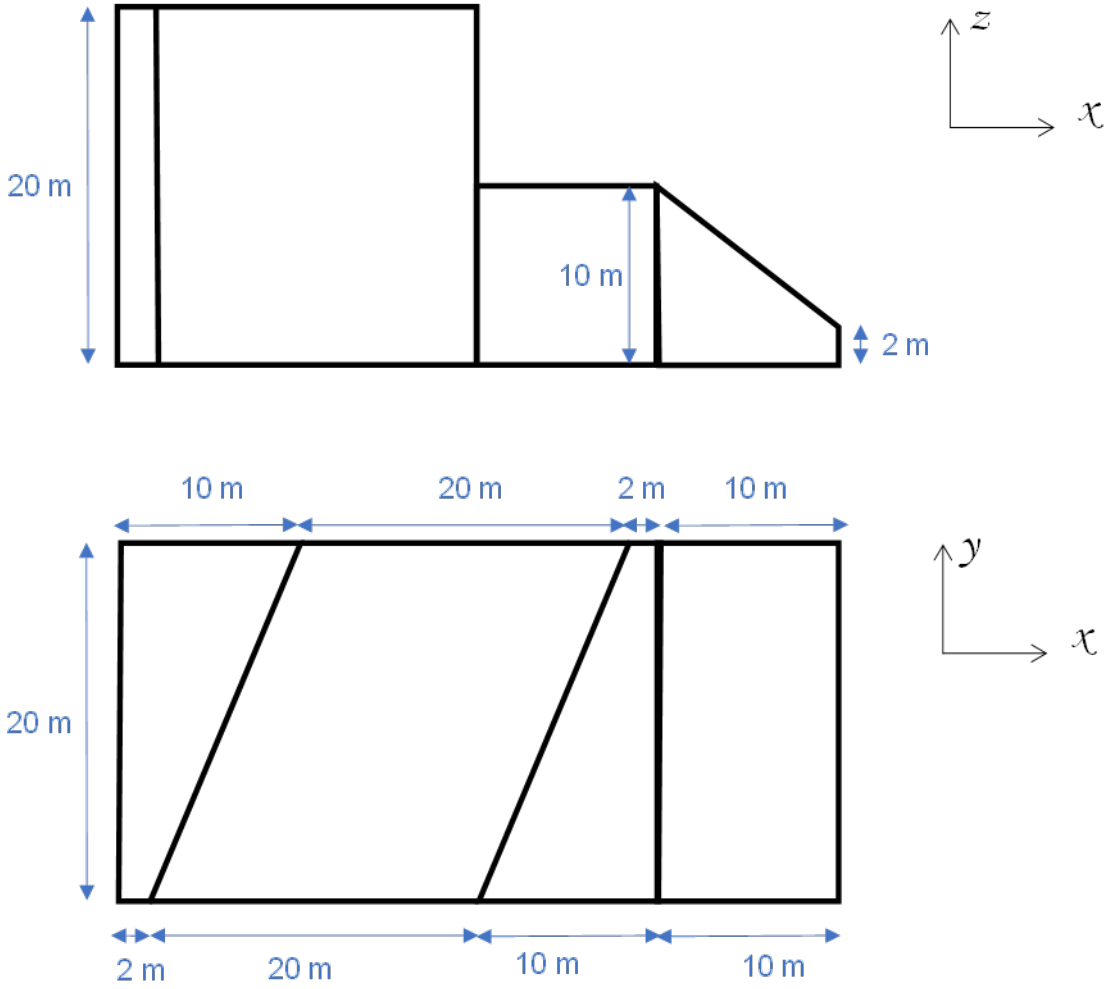

Figure 11. Simple non-cuboid geometry shown in the a) $x-z$ and b) $x-y$ planes

Table 32. Non-Cuboid: Spatial Volume parameter values (m^3)

Compartment	AMBER (Windows)	AMBER (Linux)	Analytic
Comp1	2.40000E+3	2.40000E+3	2.40000E+3
Comp2	8.00000E+3	8.00000E+3	8.00000E+3
Comp3	1.20000E+3	1.20000E+3	1.20000E+3
Comp4	1.20000E+3	1.20000E+3	1.20000E+3

Table 33. Non-Cuboid: Spatial Transfer Area parameter values (m^2)

Transfer	AMBER (Windows)	AMBER (Linux)	Analytic
Comp1_TO_Comp2	4.30813E+2	4.30813E+2	4.30813E+2
Comp2_TO_Comp3	2.15407E+2	2.15407E+2	2.15407E+2
Comp3_TO_Comp4	2.00000E+2	2.00000E+2	2.00000E+2

Table 34. Non-Cuboid: Spatial Transfer Distance parameter values (m)

Transfer	AMBER (Windows)	AMBER (Linux)	Analytic
Comp1_TO_Comp2	1.24829E+1	1.24829E+1	1.24829E+1
Comp1_TO_Comp3	1.24829E+1	1.24829E+1	1.24829E+1
Comp3_TO_Comp4	7.33333E+00	7.33333E+00	7.33333E+00

Table 35. Non-Cuboid: Spatial Top Area parameter values (m^2)

Compartment	AMBER (Windows)	AMBER (Linux)	Analytic
Comp1	1.2000E+2	1.2000E+2	1.2000E+2
Comp2	4.0000E+2	4.0000E+2	4.0000E+2
Comp3	1.2000E+2	1.2000E+2	1.2000E+2
Comp4	2.56125E+2	2.56125E+2	2.56125E+2

11 Pressure Tests

A further requirement of the AMBER 6.8 verification is pressure testing, 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.

11.1 Transfer Rates

A simple case, *PressureTest_TransferRate.cse*, was set up to investigate whether a maximum limit is encountered for 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 1.3E+154 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 Section 11.4 below).

11.2 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 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.

11.3 Contaminants and Decays

A 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 was 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.

11.4 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 1E+308, the values were stored fine (regardless of units). However, in Windows, 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 1E+308. This is because the software saves values to double-precision, and 1E+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.

11.5 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 $\sin^2(t)$ mol y^{-1}, keeping the amount of contaminant in this compartment relatively constant, oscillating around $\sim$0.5 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 1E+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 12. For values of 1E+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 yellow line in Figure 12.

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.

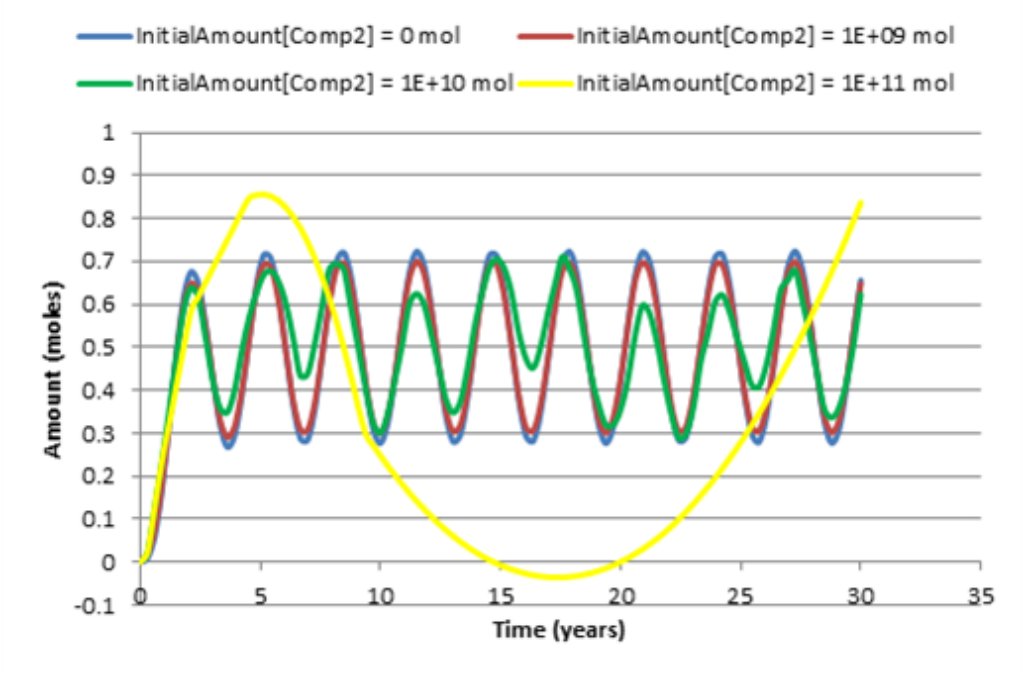

Figure 12. Solver Tolerance Test Results showing Calculated Amount in Compartment 1 with Deferring Initial Amounts in Compartment 2

12 AMBER 6.8 Targetted Tests

For the AMBER 6.8 release, specific targeted testing has been carried out for all the functionalities and issues referred to in the AMBER 6.8 release note (Quintessa, 2025c). Those issues that are relevant to calculations and results are listed below.

- Calculation run time for spatial vs non-spatial models.
- Treatment of missing values.
- Use of user units with Availability Schemes.
- Values which are $<$ 1E-03 or $\geq$ 1E+04 will be displayed using scientific notation.
- Derived parameters used in solver inputs now invalidate the calculation when modified.

All tests were passed in a Windows 11 operating system.

13 Conclusions

The wide-ranging set of test cases documented here verifies the correct functioning of AMBER 6.8 in both deterministic and probabilistic modes. Further, the outputs calculated by AMBER 6.8 as part of these tests have been compared against those from a previous AMBER release, in this instance AMBER 6.7, with the results reported in Appendix A.

These, together with the extensive user interface testing conducted for AMBER 6.8 and the continuous testing that the software 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 to the AMBER support team (contact details below) so that it can be investigated and, if necessary, corrected in subsequent versions.

AMBER Support Team:
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Telephone: +44 (0)1925 885956
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The Hub
14 Station Road
Henley-on-Thames
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United Kingdom
Website: https://www.quintessa.org/amber

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A Appendix: Verification of AMBER 6.8 Outputs Versus AMBER 6.7 Outputs

This appendix contains summary tables demonstrating a verification of the outputs calculated using AMBER 6.8 against those calculated for the previous release (AMBER 6.7) for the validation tests undertaken in the main report.

Consideration was given to both Windows and Linux installations for all the test cases. For the simple tests cases (Appendix A.1) results are presented for both Windows and Linux installations. For all other tests, the results from the Windows 11 installations are presented only, although it is noted here that the results from running the test cases through AMBER 6.8 on Linux were identical to those when running the cases through AMBER 6.7 on Linux.

A.1 Simple Test Cases

Table A.1. Comparison of SN2 Results with AMBER 6.7 and AMBER 6.8 (moles) – Windows installation

Compartment	Contaminant	Time	AMBER (6.7)		AMBER (6.8)	
			Laplace Solver	Time-step Solver	Laplace Solver	Time-step Solver
A	Nuc1	10	9.51191	9.51191	9.51191	9.51191
A	Nuc2	10	0.00466821	0.00466821	0.00466821	0.00466821
B	Nuc1	10	0.481807	0.481807	0.481807	0.481807
B	Nuc2	10	0.000137849	0.000137849	0.000137849	0.000137849
C	Nuc1	10	0.00128305	0.00128305	0.00128305	0.00128305
C	Nuc2	10	2.97307E-5	2.97310E-5	2.97307E-5	2.97310E-5
A	Nuc1	100	45.5501	45.5501	45.5501	45.5501
A	Nuc2	100	0.220230	0.220229	0.220230	0.220229
B	Nuc1	100	4.09113	4.09114	4.09113	4.09114
B	Nuc2	100	0.0188336	0.0188335	0.0188336	0.0188335
C	Nuc1	100	0.0249555	0.0249547	0.0249555	0.0249547
C	Nuc2	100	0.00142203	0.00142206	0.00142203	0.00142206

Table A.2. Comparison of SN2 Results with AMBER 6.7 and AMBER 6.8 (moles) – Linux installation

Compartment	Contaminant	Time	AMBER (6.7)		AMBER (6.8)	
			Laplace Solver	Time-step Solver	Laplace Solver	Time-step Solver
A	Nuc1	10	9.51191	9.51191	9.51191	9.51191
A	Nuc2	10	0.00466821	0.00466821	0.00466821	0.00466821
B	Nuc1	10	0.481807	0.481807	0.481807	0.481807
B	Nuc2	10	0.000137849	0.000137849	0.000137849	0.000137849
C	Nuc1	10	0.00128305	0.00128305	0.00128305	0.00128305
C	Nuc2	10	2.97307E-5	2.97310E-5	2.97307E-5	2.97310E-5
A	Nuc1	100	45.5501	45.5501	45.5501	45.5501
A	Nuc2	100	0.220230	0.220229	0.220230	0.220229
B	Nuc1	100	4.09113	4.09114	4.09113	4.09114
B	Nuc2	100	0.0188336	0.0188335	0.0188336	0.0188335
C	Nuc1	100	0.0249555	0.0249547	0.0249555	0.0249547
C	Nuc2	100	0.00142203	0.00142206	0.00142203	0.00142206

A.2 Simple Biosphere Model

Table A.3. Comparison of AMBER 6.7 and AMBER 6.8 Amounts (Bq) for Level1B

	AMBER 6.7: Amount (Bq)			AMBER 6.8: Amount (Bq)		
Time	**1**	**1000**	**100000**	**1**	**1000**	**100000**
Nuclide	**Compartment: Water**					
C14	4.67E+3	2.71E+3	2.20E-3	4.67E+3	2.71E+3	2.20E-3
U235	3.42E+0	9.69E+0	7.56E+0	3.42E+0	9.69E+0	7.56E+0
Pa231	7.25E-5	2.32E-1	6.58E+0	7.25E-5	2.32E-1	6.58E+0
Ac227	1.14E-6	2.16E-1	6.19E+0	1.14E-6	2.16E-1	6.19E+0
Nuclide	**Compartment: Sediment**					
C14	1.20E+3	3.87E+3	3.14E-3	1.20E+3	3.87E+3	3.14E-3
U235	8.70E-1	1.08E+1	8.46E+0	8.70E-1	1.08E+1	8.46E+0
Pa231	1.63E-5	2.62E-1	7.48E+0	1.63E-5	2.62E-1	7.48E+0
Ac227	2.30E-7	2.08E-1	6.00E+0	2.30E-7	2.08E-1	6.00E+0
Nuclide	**Compartment: TopSoil**					
C14	1.80E+6	2.76E+9	5.11E+3	1.80E+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	4.62E+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	2.00E+6	6.81E+7
Ac227	5.42E-2	2.00E+6	7.12E+7	5.42E-2	2.00E+6	7.12E+7

Table A.4. Comparison of AMBER 6.7 and AMBER 6.8 Doses for the U-235 decay chain for Level1B

	AMBER 6.7: Dose (Sv/y)			AMBER 6.8: Dose (Sv/y)		
Time	**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	1.2E-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	3.9E-14	4.1E-9	4.8E-9

Table A.5. Comparison of AMBER 6.7 and AMBER 6.8 Mean Stochastic Results for Level1B

Time	**AMBER 6.7: Total Dose (Sv/y)**		**AMBER 6.8: Total Dose (Sv/y)**	
	C14	**U235 Chain**	**C14**	**U235 Chain**
1	1.53E-7	2.30E-11	1.53E-7	2.30E-11
3	6.92E-7	2.95E-11	6.92E-7	2.95E-11
10	2.79E-6	8.94E-11	2.79E-6	8.94E-11
30	8.70E-6	4.36E-10	8.70E-6	4.36E-10
100	2.79E-5	2.67E-9	2.79E-5	2.67E-9
300	7.15E-5	1.57E-8	7.15E-5	1.57E-8
1000	1.40E-4	1.29E-7	1.40E-4	1.29E-7
3000	1.15E-4	8.92E-7	1.15E-4	8.92E-7
10000	2.56E-5	5.96E-6	2.56E-5	5.96E-6
30000	1.12E-6	2.03E-5	1.12E-6	2.03E-5
100000	9.23E-11	2.05E-5	9.23E-11	2.05E-5
300000	*	3.12E-6	*	3.12E-6
1000000	*	2.03E-7	*	2.03E-7

A.3 Solubility Limited Case

Table A.6. Comparison of AMBER 6.7 and AMBER 6.8 Maximum Toxicity

Nuclide	AMBER 6.7		AMBER 6.8	
	Maximum Toxicity (-)	Time of Occurrence	Maximum Toxicity (-)	Time of Occurrence
C14	2.72E+1	300	2.72E+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	3.47E+3	300
Nb94	2.22E+4	300	2.22E+4	300
Tc99	3.17E-1	300	3.17E-1	300
Sn126	3.33E+1	300	3.33E+1	300
I129	5.35E+1	300	5.35E+1	300
Cs135	4.41E+0	300	4.41E+0	300
Cs137	8.66E+3	300	8.66E+3	300
Pb210	7.14E+4	300	7.14E+4	300
Ra226	2.52E+3	300	2.52E+3	300
Ac227	2.87E+1	300000	2.87E+1	300000
Th229	7.31E+1	34756	7.31E+1	34756
Th230	2.21E+0	406040	2.21E+0	406040
Pa231	2.02E+1	300000	2.02E+1	300000
Np237	1.68E+1	3000	1.68E+1	3000
Pu238	6.94E-1	300	6.94E-1	300
Pu239	1.33E+1	40944.8	1.33E+1	40944.8
Pu240	9.28E+0	300	9.28E+0	300
Pu242	7.32E-1	269554	7.32E-1	269554
Am241	1.28E+3	300	1.28E+3	300
Am242m	9.64E-1	300	9.64E-1	300
Am243	4.11E+0	1311.13	4.11E+0	1311.13

Table A.7. Comparison of AMBER 6.7 and AMBER 6.8 Leach Rates (y^{-1})

Element	AMBER 6.7		AMBER 6.8	
	Initial Leach Rate	Maximum Leach Rate	Initial Leach Rate	Maximum Leach Rate
H	8.0E-3	8.0E-3	8.0E-3	8.0E-3
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	7.5E-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

A.4 Langmuir Availability

Table A.8. AMBER 6.7 and AMBER 6.8 Results for Simple and Shared Langmuir Schemes (moles)

Time	Simple Langmuir Model			Time	Shared Langmuir Model			
	AMBER 6.7	AMBER 6.8			AMBER 6.7		AMBER 6.8	
					A	B	A	B
0	1.000E+0	1.000E+0		0	1.00000	2.00000	1.00000	2.00000
1	9.891E-1	9.891E-1		1	0.99229	1.98730	0.99229	1.98730
2	9.782E-1	9.782E-1		2	0.98466	1.97468	0.98466	1.97468
5	9.465E-1	9.465E-1		5	0.96226	1.93739	0.96226	1.93739
10	8.958E-1	8.958E-1		10	0.92646	1.87702	0.92646	1.87702
20	8.025E-1	8.025E-1		20	0.86027	1.76267	0.86027	1.76267
50	5.770E-1	5.770E-1		50	0.69876	1.46548	0.69876	1.46548
100	3.329E-1	3.329E-1		100	0.52012	1.09340	0.52012	1.09340
200	1.108E-1	1.108E-1		200	0.34989	0.65116	0.34989	0.65116
500	4.086E-3	4.086E-3		500	0.26256	0.26215	0.26256	0.26215
1000	1.669E-5	1.669E-5		1000	0.26317	0.20302	0.26317	0.20302
1200	1.849E-6	1.849E-6		2000	0.26365	0.20081	0.26365	0.20081
1500	6.808E-8	6.808E-8		5000	0.26365	0.20081	0.26365	0.20081
2000	2.761E-10	2.761E-10		10000	0.26365	0.20081	0.26365	0.20081

A.5 Probability Distributions

Table A.9. Summary Statistics for Uniform Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	1.0001	1.0002	1.0001	1.0002
25%	1.5046	1.5000	1.5046	1.5000
50%	2.0113	2.0000	2.0113	2.0000
Mean	2.0000	2.0000	2.0000	2.0000
75%	2.4922	2.5000	2.4922	2.5000
Max	2.9999	3.0000	2.9999	3.0000

Table A.10. Summary Statistics for Log Uniform Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	1.0001E-6	1.0007E-6	1.0001E-6	1.0007E-6
25%	1.0493E-5	1.0004E-5	1.0493E-5	1.0004E-5
50%	9.7388E-5	9.9990E-5	9.7388E-5	9.9990E-5
Mean	1.0794E-3	1.0856E-3	1.0794E-3	1.0856E-3
75%	9.8133E-4	9.9940E-4	9.8133E-4	9.9940E-4
Max	9.9994E-3	9.9971E-3	9.9994E-3	9.9971E-3

Table A.11. Summary Statistics for Gaussian Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	2.9001	1.7104	2.9001	1.7104
25%	8.6511	8.6510	8.6511	8.6510
50%	10.0215	10.0001	10.0215	10.0001
Mean	10.0161	10.0000	10.0161	10.0000
75%	11.3774	11.3486	11.3774	11.3486
Max	17.7345	17.9078	17.7345	17.9078

Table A.12. Summary Statistics for Log Gaussian Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	0.13431	0.11091	0.13431	0.11091
25%	202.55	211.59	202.55	211.59
50%	983.65	1000.1	983.65	1000.1
Mean	1.2347E+4	1.3805E+4	1.2347E+4	1.3805E+4
75%	4838.3	4725.2	4838.3	4725.2
Max	1.9748E+6	7.8770E+6	1.9748E+6	7.8770E+6

Table A.13. Summary Statistics for Truncated Gaussian Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	8.0000	8.0006	8.0000	8.0006
25%	9.3329	9.3292	9.3329	9.3292
50%	10.4068	10.3968	10.4068	10.3968
Mean	10.5612	10.5656	10.5612	10.5656
75%	11.5997	11.6034	11.5997	11.6034
Max	15.9799	15.9871	15.9799	15.9871

Table A.14. Summary Statistics for Triangular Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	11.0429	11.0047	11.0429	11.0047
25%	12.7082	12.7322	12.7082	12.7322
50%	13.4380	13.4496	13.4380	13.4496
Mean	13.3255	13.3333	13.3255	13.3333
75%	14.0168	13.9999	14.0168	13.9999
Max	14.9861	14.9861	14.9861	14.9861

Table A.15. Summary Statistics for Log-Triangular Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	10.071	10.030	10.071	10.030
25%	75.525	73.455	75.525	73.455
50%	188.81	185.34	188.81	185.34
Mean	621.21	611.12	621.21	611.12
75%	607.38	596.05	607.38	596.05
Max	9387.0	9715.8	9387.0	9715.8

Table A.16. Summary Statistics for Beta Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	-4.0000	-4.0000	-4.0000	-4.0000
25%	-3.9214	-3.9218	-3.9214	-3.9218
50%	-3.6600	-3.6737	-3.6600	-3.6737
Mean	-3.4946	-3.5000	-3.4946	-3.5000
75%	-3.1839	-3.1944	-3.1839	-3.1944
Max	-2.0073	-2.0051	-2.0073	-2.0051

Table A.17. Summary Statistics for Log Beta Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	1.0000E-4	1.0000E-4	1.0000E-4	1.0000E-4
25%	1.1931E-4	1.1972E-4	1.1931E-4	1.1972E-4
50%	2.0787E-4	2.1202E-4	2.0787E-4	2.1202E-4
Mean	7.3186E-4	7.3225E-4	7.3186E-4	7.3225E-4
75%	6.3210E-4	6.3922E-4	6.3210E-4	6.3922E-4
Max	9.8269E-3	9.8643E-3	9.8269E-3	9.8643E-3

Table A.18. Summary Statistics for General CDF Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	1.0011	1.0004	1.0011	1.0004
25%	1.9858	2.0001	1.9858	2.0001
50%	4.0488	4.0004	4.0488	4.0004
Mean	4.3795	4.3750	4.3795	4.3750
75%	7.0030	7.0000	7.0030	7.0000
Max	8.0000	7.9999	8.0000	7.9999

Table A.19. Summary Statistics for Log General CDF Distribution

	AMBER 6.7		AMBER 6.8	
	Monte Carlo	**Latin Hypercube**	**Monte Carlo**	**Latin Hypercube**
Min	0.1000	0.1000	0.1000	0.1000
25%	0.6606	0.6814	0.6606	0.6814
50%	2.4730	2.5119	2.4730	2.5119
Mean	6.4095	6.3871	6.4095	6.3871
75%	7.9124	7.9437	7.9124	7.9437
Max	39.7915	39.7980	39.7915	39.7980

A.6 Correlation Checks

Here consideration is given as to whether the correlation coefficients calculated in AMBER 6.8 are similar to those calculated in AMBER 6.7 for the same two case files.

Table A.20. Standard and Ranked Correlation Coefficients in Independent Sampling Case for AMBER 6.7 and AMBER 6.8

Statistic	AMBER 6.7		AMBER 6.8	
	Monte Carlo	Latin Hypercube	Monte Carlo	Latin Hypercube
Standard correlation coefficient	-0.0013473	-0.0072046	-0.0013473	-0.0072046
Rank correlation coefficient	-0.00263604	-0.00443935	-0.00263604	-0.00443935

Table A.21. Matrix of Rank Correlation Coefficients for AMBER 6.7 and AMBER 6.8

AMBER 6.7					
Parameter	**Ppt**	**Irrig**	**RunOff**	**Kd**	**CF_Plant**
Ppt	1	-0.9070	0.8075	-1e-005	-0.0013
Irrig	-0.9070	1	-0.8536	-0.0005	0.0014
RunOff	0.8075	-0.8536	1	-0.0022	-0.0005
Kd	-1e-005	-0.0005	-0.0022	1	-0.6913
CF_Plant	-0.0013	0.0014	-0.0005	-0.6913	1
AMBER 6.8					
Parameter	**Ppt**	**Irrig**	**RunOff**	**Kd**	**CF_Plant**
Ppt	1	-0.9070	0.8075	-1e-005	-0.0013
Irrig	-0.9070	1	-0.8536	-0.0005	0.0014
RunOff	0.8075	-0.8536	1	-0.0022	-0.0005
Kd	-1e-005	-0.0005	-0.0022	1	-0.6913
CF_Plant	-0.0013	0.0014	-0.0005	-0.6913	1

A.7 Spatial Parameter Tests

Table A.22. ISAM Vault Test Case Spatial Parameters: SpatialVolume (m^3)

Compartment	AMBER 6.7	AMBER 6.8
Aquifer 1	1.07100E+5	1.07100E+5
Aquifer 2	1.89000E+4	1.89000E+4
Brown Sand 1	9.99600E+4	9.99600E+4
Brown Sand 3	1.03530E+5	1.03530E+5
Clay 1	9.63900E+4	9.63900E+4
Clay 3	9.28200E+4	9.28200E+4
Granite 1	1.16025E+5	1.16025E+5
Waste	3.21300E+5	3.21300E+5

Table A.23. ISAM Vault Test Case Spatial Parameters: SpatialTransferArea (m^2)

Transfer	AMBER 6.7	AMBER 6.8
Abstraction (Well – Sink)	0.00000E+0	0.00000E+0
Disp_back 1 (Aquifer 1 – Aquifer 2)	6.30000E+2	6.30000E+2
Leaching (Waste – Concrete Base)	3.57000E+4	3.57000E+4

Table A.24. ISAM Vault Test Case Spatial Parameters: SpatialTransferDistance (m)

Transfer	AMBER 6.7	AMBER 6.8
Disp_back 1 (Aquifer 1 – Aquifer 2)	1.00000E+2	1.00000E+2
Disp_back2	3.00000E+1	3.00000E+1
Disp_back3	3.00000E+1	3.00000E+1
Disp_back4	3.00000E+1	3.00000E+1
Leaching (Waste – Concrete Base)	4.65000E+0	4.65000E+0
Unsat_flow1	1.50000E+0	1.50000E+0
Unsat_flow11	3.25000E+0	3.25000E+0
Unsat_flow19	3.15000E+0	3.15000E+0

Table A.25. ISAM Vault Test Case Spatial Parameters: SpatialTopArea (m^2)

Compartment	AMBER 6.7	AMBER 6.8
Aquifer 1	3.5700E+4	3.5700E+4
Aquifer 2	6.300E+3	6.300E+3
Brown Sand 1	3.5700E+4	3.5700E+4
Brown Sand 3	3.5700E+4	3.5700E+4
Clay 1	3.5700E+4	3.5700E+4
Clay 3	3.5700E+4	3.5700E+4
Granite 1	3.5700E+4	3.5700E+4
Waste	3.5700E+4	3.5700E+4

Table A.26. Non-Cuboid Geometry Case Spatial Parameters: SpatialVolume (m^3)

Compartment	AMBER 6.7	AMBER 6.8
Comp1	2.40000E+3	2.40000E+3
Comp2	8.00000E+3	8.00000E+3
Comp3	1.20000E+3	1.20000E+3
Comp4	1.20000E+3	1.20000E+3

Table A.27. Non-Cuboid Geometry Case Spatial Parameters: SpatialTransferArea (m^2)

Transfer	AMBER 6.7	AMBER 6.8
Comp1_TO_Comp2	4.30813E+2	4.30813E+2
Comp2_TO_Comp3	2.15407E+2	2.15407E+2
Comp3_TO_Comp4	2.00000E+2	2.00000E+2

Table A.28. Non-Cuboid Geometry Case Spatial Parameters: SpatialTransferDistance (m)

Transfer	AMBER 6.7	AMBER 6.8
Comp1_TO_Comp2	1.24829E+1	1.24829E+1
Comp1_TO_Comp3	1.24829E+1	1.24829E+1
Comp3_TO_Comp4	7.33333E+00	7.33333E+00

Table A.29. Non-Cuboid Geometry Case Spatial Parameters: SpatialTopArea (m^2)

Compartment	AMBER 6.7	AMBER 6.8
Comp1	1.2000E+2	1.2000E+2
Comp2	4.0000E+2	4.0000E+2
Comp3	1.2000E+2	1.2000E+2
Comp4	2.56125E+2	2.56125E+2