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Comments on the samples of the Modelling Guideline

Aim and description

The aim of this report is to reflect the examples of the Modelling Guideline and document comments and deviations of the example description and the corresponding results. The concentration c_{ref} in the results of the examples are taken from the corresponding example of the guideline.

The SAFE+ Algorithmics GmbH builds the numerical algorithm migraSIM [1] for the simulation of migrating substances from polymers to drinking water or food. migraSIM is used for the simulated concentration c. The simulated concentration c is compared to c_{ref} by the *relative deviation* d_r, computed as follows:

$$d_r = \left(\frac{c}{c_{\text{ref}}} - 1\right) \cdot 100\,\% \qquad (1)$$

The input value *(additional) radius* (see example 4 and later) refers to the cylindric coordinates used for the simulation and describes the radial thickness of the layer, i. e. the length which is added to the radius of the layers below. The layers are noted form the outer to the inner. The mass of the migrant in the water is denoted by m. The partition coefficient refers to the columns the layer before the line in which it is noted and the layer in the line in which it is noted.

[1] This report includes 12 pages. A partial publication of the report requires the prior written consent of the contractor. The test and/or calculation results refer solely on the samples and/or information provided by the customer and the tested and/or calculated parameters. Reference samples or sample residues are stored for a period of 6 month as far as possible and if no deviating agreement with the contractor exists and disposed of after.

1 Example cold water test for monolayer plastic plate

layer	material	thickness	density
L1	PP	0.2 cm	0.905 $\frac{g}{cm^3}$
L2	water	2.0 cm	0.997 $\frac{g}{cm^3}$
contact area O		816 cm^2	
volume V		1632 cm^3	
ratio $\frac{O}{V}$		5 $\frac{1}{dm}$	

Table 1: matrix example 1

migrant	Butylhydroxytoluol		
layer	initial mass fraction	diffusion coefficient	partition coefficient
L1	1000 $\frac{mg}{kg}$	$2.42 \cdot 10^{-11}$ $\frac{cm^2}{s}$	-
L2	0.0 $\frac{\mu g}{kg}$	$6.5 \cdot 10^{-05}$ $\frac{cm^2}{s}$	1750 $\frac{mg/l}{mg/l}$

Table 2: parameters of migrant of example 1

time day	m(PP) mg	m(water) mg	c(water) µg/l	c_{ref}(water) µg/l	d_r %
0	147.696	0	0	-	-
1	147.199	0.497	305	305	0.00
4	146.664	0.535	328	328	0.00
7	146.184	0.480	294	294	0.00
10	145.748	0.436	267	267	0.00
14	145.315	0.433	265	265	0.00
17	144.932	0.384	235	235	0.00
21	144.548	0.384	235	235	0.00
24	144.204	0.344	211	211	0.00
28	143.856	0.348	213	213	0.00
31	143.541	0.314	192	192	0.00
mass deviation at the of the simulation $-5.8 \cdot 10^{-6}$ %.					

Table 3: result of migration of example 1

Deviation from the Modelling Guideline The density of the water is specified with 0.988 $\frac{g}{cm^3}$ in the guideline. But the result can only reproduced with the density 0.997 $\frac{g}{cm^3}$.

2 Example cold water test for monolayer epoxid resin plate

layer	material	thickness	density
L1	EP-H	0.1 cm	1.250 $\frac{g}{cm^3}$
L2	water	2 cm	0.997 $\frac{g}{cm^3}$
contact area O		808 cm^2	
volume V		1616 cm^3	
ratio $\frac{O}{V}$		5 $\frac{1}{dm}$	

Table 4: matrix example 2

migrant	Di-n-octylzinndilaurat		
layer	initial mass fraction	diffusion coefficient	partition coefficient
L1	200 $\frac{mg}{kg}$	$1.00 \cdot 10^{-15}$ $\frac{cm^2}{s}$	-
L2	0 $\frac{mg}{kg}$	$6.50 \cdot 10^{-07}$ $\frac{cm^2}{s}$	10 000 $\frac{mg/l}{mg/l}$

Table 5: parameters of migrant of example 2

time day	m(EP-H) mg	m(water) mg	c(water) µg/l	c_{ref}(water) µg/l	d_r %
0	20.200	0.00000	0	0	-
1	20.199	0.00149	0.92	0.94	-2.13
4	20.197	0.00179	1.11	1.13	-1.77
7	20.195	0.00129	0.80	0.83	-3.61
10	20.194	0.00106	0.66	0.67	-1.49
14	20.193	0.00116	0.72	0.72	0.00
17	20.192	0.00082	0.51	0.51	0.00
21	20.191	0.00094	0.58	0.58	0.00
24	20.191	0.00069	0.43	0.43	0.00
28	20.190	0.00081	0.50	0.50	0.00
31	20.189	0.00060	0.37	0.37	0.00
mass deviation at the of the simulation $-6.7 \cdot 10^{-6}$ %.					

Table 6: result of migration of example 2

Deviation from the Modelling Guideline The density of the water is specified with 0.988 $\frac{g}{cm^3}$ in the guideline. But the result can only reproduced with the density 0.997 $\frac{g}{cm^3}$.

3 Example cold water test for monolayer elastomer plate

layer	material	thickness	density
L1	EPDM	0.2 cm	$1.095\,\frac{g}{cm^3}$
L2	water	2 cm	$0.988\,\frac{g}{cm^3}$
contact area O		$816\,cm^2$	
volume V		$1632\,cm^3$	
ratio $\frac{O}{V}$		$5\,\frac{1}{dm}$	

Table 7: matrix example 3

migrant	Dicumylperoxid		
layer	initial mass fraction	diffusion coefficient	partition coefficient
L1	$20\,000\,\frac{mg}{kg}$	$6.00 \cdot 10^{-08}\,\frac{cm^2}{s}$	-
L2	$0\,\frac{mg}{kg}$	$3.60 \cdot 10^{-05}\,\frac{cm^2}{s}$	$15\,000\,\frac{mg/l}{mg/l}$

Table 8: parameters of migrant of example 3

time day	m(EPDM) mg	m(water) mg	c(water) µg/l	c_{ref}(water) µg/l	d_r %
0	3574.080	0	0	0	-
1	3571.984	2.096	1284	1284	0.00
4	3569.611	2.373	1454	1453	0.07
7	3567.239	2.372	1453	1451	0.14
10	3564.869	2.370	1452	1449	0.21
14	3562.495	2.374	1455	1450	0.34
17	3560.128	2.367	1450	1445	0.35
21	3557.757	2.371	1453	1446	0.48
24	3555.393	2.364	1448	1441	0.49
28	3553.025	2.368	1451	1442	0.62
31	3550.665	2.361	1447	1437	0.70
mass deviation at the of the simulation $-8.2 \cdot 10^{-6}$ %.					

Table 9: result of migration of example 3

4 Example cold water test for monolayer plastic pipe

layer	material	(additional) radius	density
L1	PVC-C	0.2 cm	1.500 $\frac{g}{cm^3}$
L2	water	0.6 cm	0.988 $\frac{g}{cm^3}$
contact area O		377 cm^2	
volume V		113.1 cm^3	
ratio $\frac{O}{V}$		33.33 $\frac{1}{dm}$	

Table 10: matrix example 4

migrant	Di-n-octylzinn-bis(isooctylthioglykolat)		
layer	initial mass fraction	diffusion coefficient	partition coefficient
L1	1000.0 $\frac{mg}{kg}$	$8.50 \cdot 10^{-17}$ $\frac{cm^2}{s}$	-
L2	0.0 $\frac{mg}{kg}$	$6.20 \cdot 10^{-07}$ $\frac{cm^2}{s}$	10 000 $\frac{mg/l}{mg/l}$

Table 11: parameters of migrant of example 4

time day	m(EPDM) mg	m(water) mg	c(water) µg/l	c_{ref}(water) µg/l	d_r %
0	131.947	0	0	0	-
1	131.945	0.00162	14.4	14.28	0.84
4	131.944	0.00174	15.4	15.36	0.26
7	131.942	0.00121	10.7	10.68	0.19
10	131.941	0.000972	8.6	8.56	0.47
14	131.940	0.00105	9.3	9.25	0.54
17	131.940	0.000736	6.5	6.51	-0.15
21	131.939	0.000836	7.4	7.39	0.14
24	131.938	0.000612	5.4	5.41	-0.18
28	131.938	0.000717	6.3	6.33	-0.47
31	131.937	0.000536	4.7	4.72	-0.42
mass deviation at the of the simulation $4.4 \cdot 10^{-6}$ %.					

Table 12: result of migration of example 4

Deviation from the Modelling Guideline The diffusion coefficient of the migrant in PVC-C is specified with $1.0 \cdot 10^{-16}$ $\frac{cm^2}{s}$ in the guideline. But the result can only reproduced with the diffusion coefficient of $8.5 \cdot 10^{-17}$ $\frac{cm^2}{s}$.

5 Example cold water test for multilayer plastic pipe

layer	material	(additional) radius	density
L3	EVOH	0.01 cm	1.150 $\frac{g}{cm^3}$
L2	PE	0.01 cm	0.9250 $\frac{g}{cm^3}$
L1	PE-Xa	0.2 cm	0.950 $\frac{g}{cm^3}$
L0	water	0.8 cm	0.977 $\frac{g}{cm^3}$
contact area O		502.7 cm^2	
volume V		201.1 cm^3	
ratio $\frac{O}{V}$		25 $\frac{1}{dm}$	

Table 13: matrix example 5

migrant	Maleinsäurenanhydrid		
layer	initial mass fraction	diffusion coefficient	partition coefficient
L3	0 $\frac{mg}{kg}$	$5.00 \cdot 10^{-14}$ $\frac{cm^2}{s}$	-
L2	100 $\frac{mg}{kg}$	$2.00 \cdot 10^{-08}$ $\frac{cm^2}{s}$	0.40 $\frac{mg/l}{mg/l}$
L1	0 $\frac{mg}{kg}$	$4.58 \cdot 10^{-09}$ $\frac{cm^2}{s}$	1.50 $\frac{mg/l}{mg/l}$
L0	0 $\frac{mg}{kg}$	0.00035 $\frac{cm^2}{s}$	0.85 $\frac{mg/l}{mg/l}$

Table 14: parameters of migrant of example 5

time day	m(EVOH) mg	m(PE) mg	m(PE-Xa) mg	m(water) mg	c(water) µg/l	$c_{ref}(Wasser)$ µg/l	d_r %
0	0.00000	0.58410	0.00000	0	0	-	-
1	0.00078	0.20998	0.37334	2.318E-13	1.153E-09	< 0.001	-
4	0.00096	0.12036	0.46260	1.846E-04	0.918	0.91	0.88
7	0.00102	0.09413	0.48454	4.234E-03	21.1	21	0.48
10	0.00105	0.08026	0.48582	1.256E-02	62.4	62.4	0.00
14	0.00108	0.06897	0.47070	2.637E-02	131.1	131	0.08
17	0.00109	0.06312	0.45238	2.417E-02	120.2	120.1	0.08
21	0.00111	0.05711	0.42537	3.300E-02	164.1	163	0.67
24	0.00112	0.05341	0.40372	2.534E-02	126.0	125.9	0.08
28	0.00113	0.04914	0.37624	3.173E-02	157.8	157.7	0.06
31	0.00113	0.04628	0.35574	2.335E-02	116.1	116	0.09
mass deviation at the of the simulation −0.0025 %.							

Table 15: result of migration of example 5

6 Example extended warm water test for multilayer plastic pipe

layer	material	(additional) radius	density
L3	EVOH	0.01 cm	1.150 $\frac{g}{cm^3}$
L2	PE	0.01 cm	0.925 $\frac{g}{cm^3}$
L1	PE-Xa	0.2 cm	0.950 $\frac{g}{cm^3}$
L0	water	0.8 cm	0.983 $\frac{g}{cm^3}$
contact area O		502.7 cm^2	
volume V		201.1 cm^3	
ratio $\frac{O}{V}$		25 $\frac{1}{dm}$	

Table 16: matrix of example 6

migrant	Maleinsäurenanhydrid		
layer	initial mass fraction	diffusion coefficient	partition coefficient
L3	0.0 $\frac{mg}{kg}$	$4.00 \cdot 10^{-12}$ $\frac{cm^2}{s}$	-
L2	100.0 $\frac{mg}{kg}$	$8.00 \cdot 10^{-08}$ $\frac{cm^2}{s}$	0.45 $\frac{mg/l}{mg/l}$
L1	0.0 $\frac{mg}{kg}$	$9.18 \cdot 10^{-08}$ $\frac{cm^2}{s}$	1.20 $\frac{mg/l}{mg/l}$
L0	0.0 $\frac{mg}{kg}$	0.00079 $\frac{cm^2}{s}$	0.50 $\frac{mg/l}{mg/l}$

Table 17: parameters of migrant example 6

t days	m(EVOH) mg	m(PE) mg	m(PE-Xa) mg	m(water) mg	c(water) µg/l	c_{ref}(water) µg/l	d_r %
0	0.000E+00	5.841E-01	0.000E+00	0.000E+00	0		
1	2.159E-03	4.906E-02	4.408E-01	9.207E-02	457.8	457.1	0.15
2	2.173E-03	3.251E-02	3.118E-01	1.455E-01	723.6	723.2	0.06
3	2.078E-03	2.238E-02	2.157E-01	1.064E-01	529.1	528.8	0.06
4	1.939E-03	1.546E-02	1.490E-01	7.378E-02	366.9	366.7	0.05
7	1.532E-03	5.608E-03	6.118E-02	9.803E-02	487.5	487.3	0.04
8	1.429E-03	4.113E-03	4.004E-02	2.274E-02	113.1	113.0	0.09
9	1.333E-03	2.865E-03	2.759E-02	1.379E-02	68.6	68.6	0.00
10	1.247E-03	1.987E-03	1.911E-02	9.445E-03	47.0	46.9	0.21
11	1.172E-03	1.379E-03	1.325E-02	6.538E-03	32.5	32.5	0.00
14	1.000E-03	5.105E-04	5.531E-03	8.761E-03	43.6	43.6	0.00
15	9.570E-04	3.777E-04	3.653E-03	2.054E-03	10.2	10.2	0.00
16	9.183E-04	2.663E-04	2.545E-03	1.258E-03	6.26	6.25	0.16
17	8.835E-04	1.877E-04	1.787E-03	8.714E-04	4.33	4.33	0.00
18	8.524E-04	1.329E-04	1.261E-03	6.116E-04	3.04	3.04	0.00

21	7.757E-04	5.388E-05	5.657E-04	8.509E-04	4.23	4.23	0.00
22	7.546E-04	4.151E-05	3.900E-04	2.092E-04	1.04	1.04	0.00
23	7.351E-04	3.095E-05	2.856E-04	1.344E-04	0.67	0.67	0.00
24	7.171E-04	2.337E-05	2.133E-04	9.792E-05	0.49	0.49	0.00
25	7.004E-04	1.799E-05	1.623E-04	7.313E-05	0.36	0.36	0.00
28	6.566E-04	9.944E-06	9.501E-05	1.191E-04	0.59	0.59	0.00
29	6.438E-04	8.563E-06	7.449E-05	3.470E-05	0.17	0.17	0.00
30	6.318E-04	7.283E-06	6.214E-05	2.570E-05	0.13	0.13	0.00
31	6.204E-04	6.387E-06	5.614E-05	4.400E-05	0.11	???	
mass deviation at the of the simulation $1.2 \cdot 10^{-5}$ %.							

Table 18: result of migration of example 6

Deviation from the Modelling Guideline The reference concentration of the cycle after 31 days is missing.

7 Example cold water test after storage for multilayer plastic pipe

Even without an explicit storage model the storage can be simulated with a very low diffusion coefficient and a very high partion coefficient for the storage period which corresponds to numerically zero migration. The diffusion coefficient is choosen to $10^{-32}\,\frac{\text{cm}^2}{\text{s}}$ and the partition coefficient is choosen to 10^8.

layer	material	(additional) radius	density
L3	EVOH	0.01 cm	$1.150\,\frac{\text{g}}{\text{cm}^3}$
L2	PE	0.01 cm	$0.925\,\frac{\text{g}}{\text{cm}^3}$
L1	PE-Xa	0.2 cm	$0.950\,\frac{\text{g}}{\text{cm}^3}$
L0	water	0.8 cm	$0.977\,\frac{\text{g}}{\text{cm}^3}$
contact area O		$502.7\,\text{cm}^2$	
volume V		$201.1\,\text{cm}^3$	
ratio $\frac{O}{V}$		$25\,\frac{1}{\text{dm}}$	

Table 19: matrix example 7

migrant	Maleinsäurenanhydrid			
layer	initial mass fraction	diffusion coefficient	partition coefficient	
L3	$0.0\,\frac{\text{mg}}{\text{kg}}$	$3.75 \cdot 10^{-14}\,\frac{\text{cm}^2}{\text{s}}$	-	storage
		$5.00 \cdot 10^{-14}\,\frac{\text{cm}^2}{\text{s}}$	-	test
L2	$100.0\,\frac{\text{mg}}{\text{kg}}$	$1.00 \cdot 10^{-08}\,\frac{\text{cm}^2}{\text{s}}$	$0.52\,\frac{\text{mg/l}}{\text{mg/l}}$	storage
		$2.00 \cdot 10^{-08}\,\frac{\text{cm}^2}{\text{s}}$	$0.40\,\frac{\text{mg/l}}{\text{mg/l}}$	test
L1	$0.0\,\frac{\text{mg}}{\text{kg}}$	$2.87 \cdot 10^{-09}\,\frac{\text{cm}^2}{\text{s}}$	$1.90\,\frac{\text{mg/l}}{\text{mg/l}}$	storage
		$4.58 \cdot 10^{-09}\,\frac{\text{cm}^2}{\text{s}}$	$1.50\,\frac{\text{mg/l}}{\text{mg/l}}$	test
L0	$0.0\,\frac{\text{mg}}{\text{kg}}$	$1.00 \cdot 10^{-32}\,\frac{\text{cm}^2}{\text{s}}$	$1.00 \cdot 10^{+08}\,\frac{\text{mg/l}}{\text{mg/l}}$	storage

		$0.00035\,\frac{cm^2}{s}$	$0.85\,\frac{mg/l}{mg/l}$	test

Table 20: parameters of migrant example 7

t days	m(EVOH) mg	m(PE) mg	m(PE-Xa) mg	m(water) mg	c(water) µg/l	c_{ref}(water µg/l	rel. deviation %
-30	0.000000	0.5841	0	0	0		
0	0.001885	0.07400	0.5082	0.00000	0		
1	0.001804	0.06366	0.4873	0.03135	155.9	155.8	0.06
4	0.001727	0.05811	0.4550	0.03796	188.8	188.7	0.05
7	0.001686	0.05470	0.4280	0.03042	151.3	151.2	0.07
10	0.001657	0.05176	0.4035	0.02742	136.4	136.3	0.07
14	0.001627	0.04810	0.3742	0.03305	164.3	164.3	0.00
17	0.001607	0.04549	0.3530	0.02377	118.2	118.1	0.08
21	0.001582	0.04222	0.3276	0.02871	142.8	142.7	0.07
24	0.001564	0.03991	0.3092	0.02073	103.1	103.0	0.10
28	0.001540	0.03702	0.2870	0.02510	124.8	124.8	0.00
31	0.001522	0.03498	0.2709	0.01814	90.2	90.2	0.00
mass deviation at the of the simulation $-0.0032\,\%$.							

Table 21: result of migration of example 7

8 Example extended warm water test after storage for multilayer plastic pipe

layer	material	(additional) radius	density
L3	EVOH	0.01 cm	$1.150\,\frac{g}{cm^3}$
L2	PE	0.01 cm	$0.925\,\frac{g}{cm^3}$
L1	PE-Xa	0.2 cm	$0.950\,\frac{g}{cm^3}$
L0	water	0.8 cm	$0.983\,\frac{g}{cm^3}$
contact area O		$502.7\,cm^2$	
volume V		$201.1\,cm^3$	
ratio $\frac{O}{V}$		$25\,\frac{1}{dm}$	

Table 22: matrix example 8

migrant	Maleinsäurenanhydrid			
layer	initial mass fraction	diffusion coefficient	partition coefficient	
L3	$0.0\,\frac{mg}{kg}$	$3.75 \cdot 10^{-14}\,\frac{cm^2}{s}$	-	storage
		$4.00 \cdot 10^{-12}\,\frac{cm^2}{s}$	-	test

L2	100.0 $\frac{mg}{kg}$	$1.00 \cdot 10^{-08}\ \frac{cm^2}{s}$	$0.52\ \frac{mg/l}{mg/l}$	storage
		$8.00 \cdot 10^{-08}\ \frac{cm^2}{s}$	$0.45\ \frac{mg/l}{mg/l}$	test
L1	0.0 $\frac{mg}{kg}$	$2.87 \cdot 10^{-09}\ \frac{cm^2}{s}$	$1.90\ \frac{mg/l}{mg/l}$	storage
		$9.18 \cdot 10^{-08}\ \frac{cm^2}{s}$	$1.20\ \frac{mg/l}{mg/l}$	test
L0	0.0 $\frac{mg}{kg}$	$1.00 \cdot 10^{-32}\ \frac{cm^2}{s}$	$1.00 \cdot 10^{+08}\ \frac{mg/l}{mg/l}$	storage
		$0.00079\ \frac{cm^2}{s}$	$0.50\ \frac{mg/l}{mg/l}$	test

Table 23: parameters of migrant of example 8

t days	EVOH mg	PE mg	PE-Xa mg	Wasser mg	c(Wasser) µg/l	c_{ref}(water) µg/l	d_r %
-30	0	0.5841	0	0	0		
0	0.001885	0.07400	0.5082	0.0000	0		
1	0.001814	0.03645	0.3531	0.1928	958.7	958.2	0.05
2	0.001821	0.02520	0.2431	0.1212	602.9	602.6	0.05
3	0.001734	0.01740	0.1677	0.0832	413.7	413.4	0.07
4	0.001614	0.01202	0.1158	0.0574	285.4	285.3	0.04
7	0.001276	0.004363	0.04760	0.0762	379.1	379	0.03
8	0.001191	0.003200	0.03115	0.0177	88	87.9	0.11
9	0.001112	0.002230	0.02147	0.0107	53.4	53.3	0.19
10	0.001042	0.001547	0.01487	0.007351	36.6	36.5	0.27
11	0.0009802	0.001074	0.01032	0.005089	25.3	25.3	0.00
14	0.0008391	0.0003981	0.004311	0.006824	33.9	33.9	0.00
15	0.0008035	0.0002947	0.002849	0.001601	8.0	8.0	0.00
16	0.0007716	0.0002080	0.001986	0.0009816	4.9	4.9	0.00
17	0.0007430	0.0001467	0.001396	0.0006802	3.4	3.4	0.00
18	0.0007172	0.0001041	0.0009865	0.0004779	2.4	2.4	0.00
21	0.0006538	4.246E-05	0.0004449	0.0006667	3.3	3.3	0.00
22	0.0006362	3.280E-05	0.0003076	0.0001645	0.82	0.82	0.00
23	0.0006200	2.455E-05	0.0002261	0.0001060	0.53	0.53	0.00
24	0.0006050	1.862E-05	0.0001695	7.750E-05	0.3854	0.38	1.42
25	0.0005911	1.440E-05	0.0001295	5.811E-05	0.29	0.29	0.00
28	0.0005546	8.078E-06	7.687E-05	9.546E-05	0.47	0.47	0.00
29	0.0005439	6.987E-06	6.060E-05	2.806E-05	0.14	0.14	0.00
30	0.0005338	5.970E-06	5.080E-05	2.091E-05	0.1	0.1	0.00
31	0.0005242	5.193E-06	4.365E-05	1.747E-05	0.08687	???	

mass deviation at the of the simulation $5.3 \cdot 10^{-5}$ %.

Table 24: result of migration of example 8

Deviation from the Modelling Guideline The reference concentration of the cycle after the 31 day is missing.

The number of significant digits of the reference concentration is to low to compare the the simulation to high accuracy. Example: day 24. with two digits $c_{(}\text{water}) = 0.3854 \approx 0.39$, $c_{\text{ref}}(\text{water} = 0.38$, results in a relative deviation of 2.63 %, but if three digits are used for $c_{(}\text{water})$ the relative deviation decrease to 1.32 %. If $c_{\text{ref}}(\text{water})$ is rounded 0.38 (Gaussian rounding or symmetric rounding; if the first not significant digit is 5 round to the even number) the relative deviation is 0 %. Second example: day 30: $c(\text{water}) = 0.1040 \approx 0.1$ and $c_ref(\text{water}) = 0.1$ (only one significant digit), i. e. $d_r = 0.0\,\%$ of the rounded value but $d_r = 3.97$ of the not rounded value.

Significant digits and rounding of the reference concentration

civil rounding [2] round numbers with the first not significant digit 1, 2, 3, 4 downwards. Round numbers with the first not significant digit 5, 6, 7, 8, 9 upwards (introduce systematic error).

scientific rounding [3] round numbers with the first not significant digit 1, 2, 3, 4 downwards. Round numbers with the first not significant digit 6, 7, 8, 9 upwards. Round numbers with the first not significant digit 5 to the even numbers (remove systematic error of civil rounding).

	c	$\text{round}_{\text{civil}}(c)$	d_r	$\text{round}_{\text{scientific}}(c)$	d_r	c_{ref}
two significant digits	1.0500	1.1	10.0 %	1.0	0.0 %	1.000
four significant digits	1.0500	1.050	5.0 %	1.050	5.0 %	1.000
	1.0005	1.001	0.1 %	1.000	0.0 %	1.000

Table 25: significant digits and rounding

The usage of four significant digits will decrease the influence of the rounding of the results. Also the guideline should suggest to use scientific rounding. This will improve the reliability of the comparison of the numerical solvers with the reference concentrations.

Remark Not every spreadsheet software uses scientific round, i. e. a post processing of the value can be distorted by rounding.

The calculations and their evaluation are limited to the information made available and are elaborated to the best of our knowledge and belief according to the state-of-art in science and technology.

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References

[1] Dieter Schuster and Rainer Brandsch. *migraSIM*. [Online; accessed 2022-03-08]. URL: https://www.saferithm.com/products/migrasim.

[2] or banking rounding

[3] also known as symmetric or gaussian rounding