Electronic Supplementary Material (ESI) for Environmental Science: Nano.

Supplementary Information: Multimedia Environmental Fate and Speciation of Engineered Nanoparticles: A probabilistic Modeling Approach

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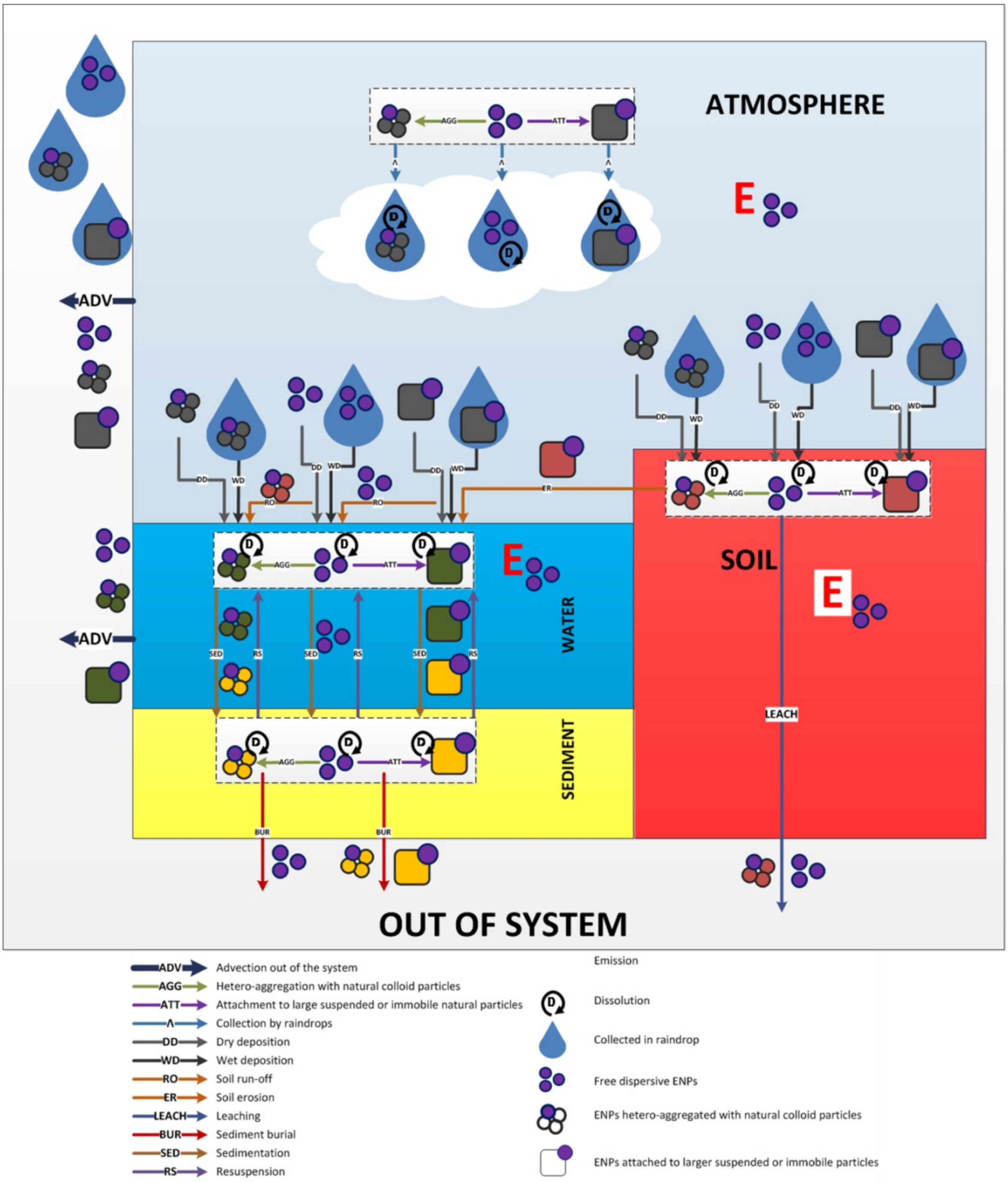
SI Chapter A: Multimedia Fate Modeling With SimpleBox4nano

Model Concept

SimpleBox4nano (SB4N) is an extension of SimpleBox, a classical multi-media mass balance model ("box model") that calculates chemical masses m (kg) in the various environmental compartments (air, water, soil, etc.) (Mackay, 2001; Van de Meent, 2011). In addition, SB4N calculates the masses of the different physical-chemical forms (species), in which ENPs can occur within each compartment: (a) freely dispersed, (b) hetero-aggregated with natural colloidal particles, or (c) attached to larger natural particles that are prone to gravitational forces in aqueous media (SI A Figure 1). The model solves mass balance equations for a steady-state situation in all compartments and species through matrix algebra (Meesters et al., 2014): $m = -A^{-1}e$. Here is e (kg.s-1) the vector of emission rates of (pristine) ENPs into the environment. The system matrix A (s-1) represents (pseudo) first-order rate constants for (a) transport between compartments (b) removal by transport out of the system (c) the rates at which ENPs are taken up in aggregates or attach to the surfaces of larger particles, and (d) the rates at which ENPs may be subjected to removal processes such as degradation and dissolution (SI A Figure 1).



SI A Figure 1. Model Concept SimpleBox4nano.

For the purpose of this study SB4N only uses one spatial scale resembling a regional environmental system as defined in REACH (ECHA, 2012) instead of the nested spatial scales. Dissolution is considered as removal of the chemical material, because after dissolution the ENP is no longer a nanoscaled solid particle that applies to the definition of an ENP (Bleeker et al, 2013; Meesters et al., 2014). Emission estimation itself is not part of SB4N's system matrix. Therefore, the emission rate needs to be obtained from other data sources in order to be used as input for the SB4N model.

Model Simplifications

The environmental behavior of ENPs is so complex that simplifications are necessary to predict their environmental fate (Praetorius et al., 2013). SB4N also employs such simplifications (Meesters et al., 2014), which are inevitable but acceptable if they can be justified scientifically (Praetorius et al., 2013).

Prior to the fate simulation the ENPs that are directly released to the environment are assumed to be in their pristine state, whereas ENPs that are released to the surface waters via the effluents of waste water treatment plants (WWTPs) are assumed to be hetero-aggregated with natural colloid particles, and ENPs emitted to soil through the application of WWTP sludge are assumed to be attached to natural coarse particles prone for gravitational settling in aqueous media. However, transformation processes such as homoaggregation, surface modification and weathering can alter the pristine state before, during or directly after release (Meesters et al., 2013; Nowack et al., 2012) Quantitative data on the release of ENPs is limited (Nowack et al., 2012), so that the extent to which ENPs are physically or chemically altered upon emission is difficult to express (Keller et al., 2013). Hence, the pristine state of ENPs is chosen as a starting point for the fate simulations, because most data on physicochemical properties of nano-CeO2, -TiO2 and -ZnO are referring to this state (Gottschalk et al., 2013a,b). The ENPs in pristine state are assumed to be in spherical shape and their mass densities to be equal to the densities of the solid states of the pure chemical of which the ENP consists. Possible influences of coatings on the ENPs' weight are assumed negligible.

Complex physical and chemical transformations reactions between ENPs and environmental matrices such as (re-)oxidation, sulfidication, phosphorization, functionalization and carbon sorption, are not explicitly simulated. Rather, these processes are implicitly included through the influence that they have on ENP dissolution rates in different aqueous media and the attachment between ENPs and natural particles (Nowack et al., 2012; Petosa et al., 2010).

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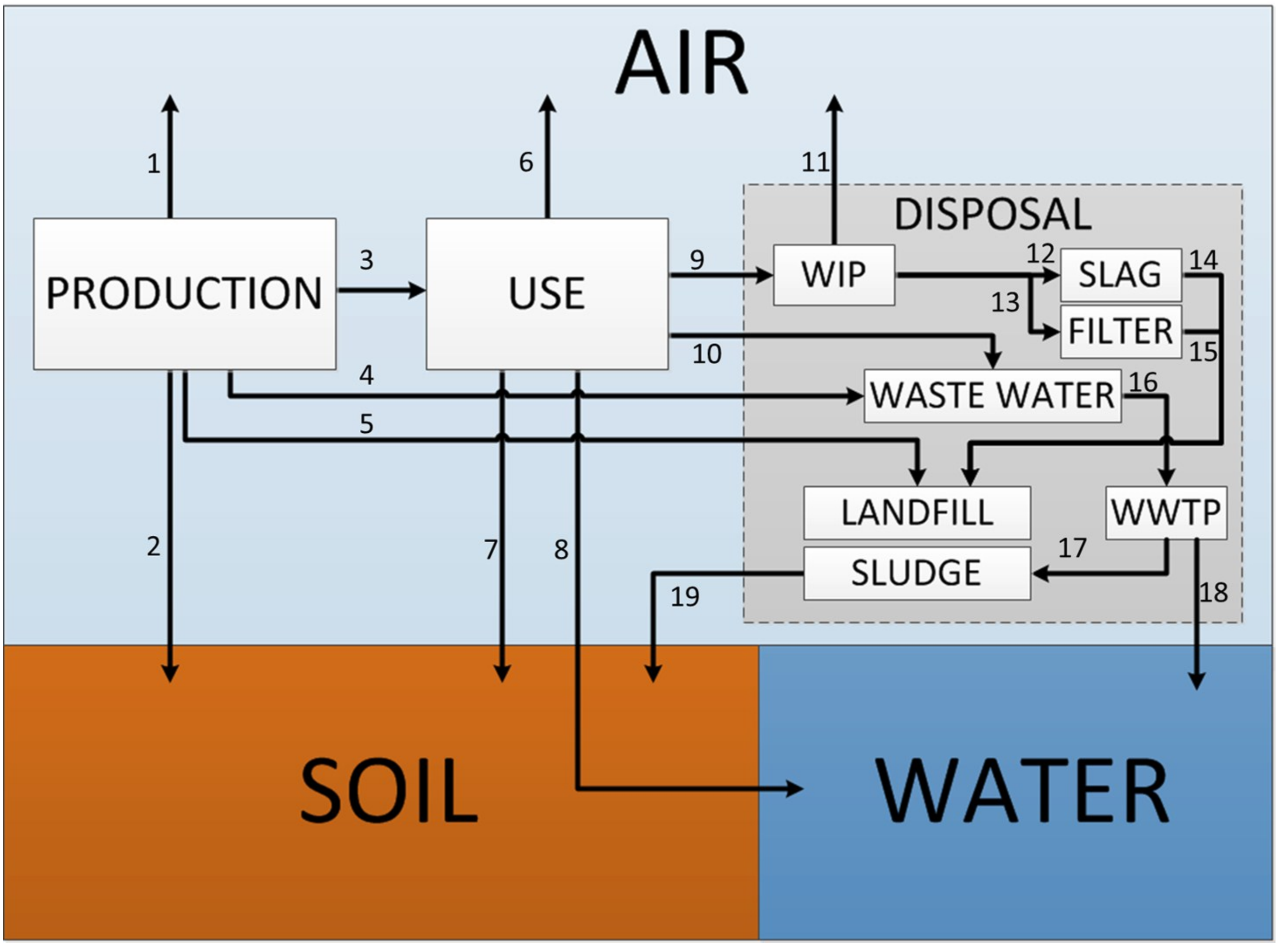
SI Chapter B: Emission Estimation



SI B Figure 1. Environmental release during different stages of the life cycle of engineered nanomaterials based on the mass flows given in Keller et al., 2013.

SI B Table 1

Nr.	Life Cycle stage	Volume Fraction (VF) to	Volume Fraction	
			Low Exposure	High Exposure
1	Production	Air	0.1 X $(1-VF_3)$	0.4 X $(1-VF_3)$
2	Production	Soil	0.001 X $(1-VF_3)$	0.02 X $(1-VF_3)$
3	Production	Use	1	0.985
4	Production	Waste Water	0.1 X $(1-VF_3)$	0.4 X $(1-VF_3)$
5	Production	Landfill	$(1-VF_3)$ X $(1-\sum VF_{1,2,4})$	
6.1	Use: Electronics & Optics*[1]	Air	5.00E-04	2.50E-03
6.2	Use: Medical*[1]	Air	2.50E-03	1.25E-02
6.3	Use: Catalysts*[1]	Air	5.00E-04	2.50E-03
6.4	Use: Cosmetics*[1]	Air	7.50E-03	9.50E-03
6.5	Use: Plastics*[1]	Air	5.00E-04	2.50E-03
6.6	Use: Energy & Environment*[1]	Air	2.50E-03	1.00E-02
6.7	Use: Coatings*[1]	Air	1.00E-03	9.00E-03
6.8	Use: Filtration*[1]	Air	0	0
6.9	Use: Textile*[1]	Air	5.00E-03	4.75E-02
6.10	Use: Composites*[1]	Air	5.00E-04	5.00E-03
6.11	Use: Automotive*[1]	Air	0	5.00E-04
6.12	Use: Aerospace*[1]	Air	0	5.00E-04
7.1	Use: Electronics & Optics*[1]	Soil	9.00E-03	4.50E-02
7.2	Use: Medical*[1]	Soil	2.50E-03	1.25E-02
7.3	Use: Catalysts*[1]	Soil	5.00E-04	2.50E-03
7.4	Use: Cosmetics*[1]	Soil	7.50E-03	9.50E-03
7.5	Use: Plastics*[1]	Soil	4.20E-02	2.10E-01
7.6	Use: Energy & Environment*[1]	Soil	4.50E-02	1.80E-01
7.7	Use: Coatings*[1]	Soil	3.50E-02	3.15E-01
7.8	Use: Filtration*[1]	Soil	5.00E-03	4.50E-02
7.9	Use: Composites*[1]	Soil	9.00E-03	9.00E-02
7.10	Use: Automotive*[1]	Soil	0	5.00E-04
7.11	Use: Aerospace*[1]	Soil	0	5.00E-04
7.12	Use: Sensors*[1]	Soil	4.75E-03	9.50E-03
7.13	Use: Packaging*[1]	Soil	4.75E-02	2.38E-01
7.14	Use: Paper and board*[1]	Soil	4.75E-02	2.38E-01
8.1	Use: Cosmetics*[1]	Water	6.00E-02	7.60E-02
8.2	Use: Coatings*[1]	Water	4.00E-03	3.60E-02
9	Use	Waste Incineration Plant (WIP)	$1-\sum VF_{6,7,8,10}$	
10.1	Electronics & Optics*[1]	Waste Water	5.00E-04	2.50E-03
10.2	Medical*[1]	Waste Water	4.50E-02	2.25E-01
10.3	Catalysts*[1]	Waste Water	9.00E-03	4.50E-02
10.4	Cosmetics*[1]	Waste Water	6.75E-01	8.55E-01
10.5	Plastics*[1]	Waste Water	2.50E-03	1.25E-02
10.6	Energy & Environment*[1]	Waste Water	2.50E-03	1.00E-02
10.7	Coatings*[1]	Waste Water	6.00E-02	5.40E-01
10.8	Filtration*[1]	Waste Water	9.50E-02	8.55E-01
10.9	Textile*[1]	Waste Water	9.50E-02	9.03E-01

10.10	Composites*1	Waste Water	5.00E-04	5.00E-03
10.11	Automotive*1	Waste Water	0.00E+00	9.00E-03
10.12	Aerospace*1	Waste Water	0.00E+00	9.00E-03
10.13	Sensors*1	Waste Water	2.50E-04	5.00E-04
10.14	Packaging*1	Waste Water	2.50E-03	1.25E-02
10.15	Paper and board*1	Waste Water	2.50E-03	1.25E-02
11	Waste: Incineration	Air	5.00E-04	1.00E-02
12	Waste: Incineration	Slag	0.5	0.01
13	Waste: Incineration	Filter	1-∑VolumeFraction$_{11,12}$	
14	Waste: Slag	Landfill	1	1
15	Waste: Filter	Landfill	1	1
16	Waste: Waste Water	Waste Water Treatment Plant	1	1
17	Waste: Waste Water Treatment	Sludge	0.25	0.003
18	Waste: Waste Water Treatment	Water	1-VolumeFraction$_{17}$	
19	Waste: Sludge Application	Soil	0.55*2	0.55*2

*1 To be multiplied with use pattern of the specific nanomaterial given in SI Table 1.2

*2 It is assumed that 55% of the EU sludge is applied to agricultural soil [Sun et al., 2014]

SI B Table 2 Use patterns for nano-CeO_2, -TiO_2, and -ZnO taken from data of Keller et al., 2013.

Use Pattern	Nano-CeO_2	Nano-TiO_2	Nano-ZnO
Electronics & Optics	0.45	0.075	0.002
Medical	0.05	0	0
Catalysts	0.25	0.001	0
Cosmetics	0	0.594	0.826
Plastics	0	0.051	0.02
Energy & Environment	0.1	0.007	0
Coatings, paints, pigments	0.15	0.143	0.15
Filtration	0	0.058	0.001
Textile	0	0.003	0
Composites	0	0.068	0.001
Automotive	0	0	0
Aerospace	0	0	0
Sensors	0	0	0
Packaging	0	0	0
Paper and board	0	0	0

SI B Table 3. Results from Monte Carlo simulation on the flow chart of Keller et al., 2013 fitted into uncertainty distributions of emission estimations. All ENPs that enter surface waters via waste water treatment plant (WWTP) effluents are assumed to be aggregated (agg) with natural colloid particles (<1000 nm). All ENPs that enter soil via application of the sludge from waste water treatment plant (WWTP) are assumed to be attached (att) to larger natural particles (>1000 nm) prone for primary sedimentation. *1 Nano-ZnO is completely removed from WWTP effluents through settling and dissolution (Lombi et al., 2012). *2 Multiplied with an uncertain factor for the amount of sludge applied, i.e. a uniform distribution with a minimum 0 (no sludge application) and maximum 1 (maximum sludge application of 55%)

Emission Fractions ($t.y^{-1}$ released)/($t.y^{-1}$ produced)	Defaults And Uncertainty Distributions Of Emission Estimations		
	Nano-CeO2	Nano-TiO2	Nano-ZnO
Free ENPs to air	**Default: 0.01** **Beta Distribution** Minimum: 0 Maximum: 0.02 Alpha: 2.72 Beta:2.86	**Default: 0.01** **Beta Distribution** Minimum: 0 Maximum: 0.02 Alpha: 5.74 Beta:10.52	**Default: 0.01** **Gamma Distribution** Location: 0.01 Scale: 0 Shape: 13.88
Free ENPs directly to surface waters	**Default: 0.05** **Uniform Distribution** Minimum: 0 Maximum: 0.01	**Default: 0.045** **Beta Distribution** Minimum: 0.04 Maximum: 0.05 Alpha: 2.07 Beta:2.15	**Default: 0.06** **Beta Distribution** Minimum: 0.05 Maximum: 0.07 Alpha: 1.64 Beta:1.65
Agg. ENPs to surface water after WWTP	**Default: 0.01** **Weibull** Location: 0 Scale: 0.01 Shape: 1.62	**Default: 0.075** **Beta Distribution** Minimum: 0.01 Maximum: 0.14 Alpha: 1.11 Beta:1.36	**Default:0** **Distribution** **0 *1**
Free ENPs directly to soil	**Default: 0.05** **Beta Distribution** Minimum: 0.02 Maximum: 0.08 Alpha: 2.24 Beta:2.18	**Default: 0.045** **Beta Distribution** Minimum: 0.02 Maximum: 0.07 Alpha: 1.38 Beta:1.36	**Default: 0.035** **Beta Distribution** Minimum: 0.01 Maximum: 0.06 Alpha: 1.05 Beta:1.05
Att. ENPs from sludge application to soil*2	**Default: 0.03** **Beta Distribution** Minimum: 0.01 Maximum: 0.05 Alpha: 1.43 Beta:1.6	**Default: 0.26** **Beta Distribution** Minimum: 0.17 Maximum: 0.35 Alpha: 4.9 Beta:6.61	**Default:10^-2.4** **10^ (Beta Distribution)** Minimum: -42 Maximum: -2.4 Alpha: 100 Beta:1.27

SI B Table 4 Estimated production volumes in Europe [Piccino et al., 2012; Sun et al., 2014]

Nanomaterial	Shape	Production Volume (t.y-1)	Ref.
Nano-CeO_2	Lognormal	Default: 55 25th percentile: 0.55 Median: 55 75th percentile: 2800	Piccino et al., 2012
Nano-TiO_2	Lognormal	Default: 10,000 Min: 246 Mode: 10,000 Max 49,373	Sun et al., 2014
Nano-ZnO	Lognormal	Default: 1600 Min: 5.5 Mode: 1600 Max: 28,000	Sun et al., 2014

Literature

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SI Chapter C: A priori characterized dissolution rates

SI C Table 1. ENP dissolution rates a priori characterized with a uniform distribution from the classification framework of Garner and Keller, 2014.

		Residence times			Dissolution Rate (s^{-1})		
ENP	Medium	Classification	Min	Max	Default	Min	Max
Nano-ZnO	Stormwater	“Weeks”	1 Week	1 Month	9.85 10^{-7}	3.710^{-7}	1.65 10^{-6}
	Freshwater	“Days”	1 Day	1 Week	8.8 10^{-6}	1.65 10^{-6}	1.16 10^{-5}
	Groundwater	“Weeks”	1 Week	1 Month	1 10^{-6}	3.710^{-7}	1.65 10^{-6}

Literature

Garner, K.L.; Keller, A.A. Emerging patterns for engineered nanomaterials in the environment: a review of fate and toxicity studies. *J. Nanopart. Res.* **2014**, *16*, 2503

SI Chapter D: A priori characterization of attachment efficiencies with simulation DLVO theory

SB4N employs the Smoluchowski equation to derive attachment rates between ENPs and the natural particles occurring as colloidal particles in soil and sediment pore waters and for both the colloidal and non-colloidal natural particles that are suspended in surface waters [Quik et al., 2011]. For attachment to the solid grains in soils and sediments, SB4N uses the particle filtration theory [Tufenkji & Elimelech, 2004]. Both of these methods obtain attachment rates by calculating a collision rate between the ENP and the natural particles, which is multiplied with a so called attachment efficiency that expresses the probability of the ENP actually attaching to the natural particle at a collision. The collision rates are derived from particle size, mass and number concentration [Meesters et al., 2014], whereas obtaining attachment efficiencies is done in a less straight forward manner [Petosa et al., 2010]. The derivation of collision rates is therefore integrated in the SB4N model, while the attachment efficiencies are needed as input parameters [Meesters et al., 2014].

Attachment efficiencies can be predicted using the Derjaguin and Landau [1941] Verwey and Overbeek [1948] (DLVO) theory, but to our knowledge, the DLVO theory has not been applied successfully to predict attachment efficiencies between ENPs and natural (colloid) particles under real, complex, and environmental conditions that are not ideal for extrapolations from laboratory conditions [Petosa et al., 2010]. Therefore, experimentally derived attachment efficiencies are preferred to use as input parameters for SB4N [Meesters et al., 2014]. In case such data is not available the DLVO theory is applied nonetheless, requiring the radius, surface charge and Hamaker constant of both the ENP and natural particle as input as well as the concentration of ions and their valence that are present in the aqueous medium(SI C Eq 1-4) [Petosa et al., 2010].

$$\alpha = \frac{\int_{0}^{\infty}\left[\exp\left(\frac{V_{VDW}}{k_b T}\right)/(\left(\frac{r_{ENP} r_{NCP}}{r_{ENP} + r_{NCP}}\right) + h)^2 dh\right]}{\int_{0}^{\infty}\left[\exp\left(\frac{V_T}{k_b T}\right)/(\left(\frac{r_{ENP} r_{NCP}}{r_{ENP} + r_{NCP}}\right) + h)^2 dh\right]}$$

Eq. 1 Calculation of attachment efficiency (α) by application of the DLVO theory (Book Lead & Smith pp 130; Petosa et al., 2010) assuming effective diameter = (r_{enp} *r_{nc})/(r_{enp} +r_{nc}) and correction for diffusive approach is negligible.

$$V_{VDW} = -\frac{A_{Hamaker(ENP,water,NCP)} \cdot r_{ENP} \cdot r_{NCP}}{6h(r_{ENP} + r_{NCP})}$$

Eq. 2 Expression for Van der Waals attraction between ENP and natural colloid (Petosa et al., 2010 , Simplified)

$$V_T = V_{VDW} + V_{EDL}$$

Eq. 3. Expression for total interaction

$$V_{EDL} = 64\pi\varepsilon_0\varepsilon_{water}\left(\frac{r_{ENP} r_{NCP}}{r_{ENP} + r_{NCP}}\right)\left(\frac{k_b T}{ze}\right)^2 tanh\left(\frac{ze\zeta_{ENP}}{4k_b T}\right) tanh\left(\frac{ze\zeta_{NCP}}{4k_b T}\right) exp(-k_{Debye} h)$$

Eq. 4. Expression for Electric Double Layer repulsion between ENP and natural colloid (Petosa et al., 2010)

SI D Table 1 Glossary of terms for a priori characterization of attachment efficiencies between engineered nanoparticles and natural counter particles through simulation of the classical DLVO theory

Symbol	Parameter	Unit
α	Attachment Efficiency	(-)
V_{VDW}	Van der Waals attraction	J
V_{EDL}	Electric Double Layer Repulsion	J
V_T	Total Interaction	J
k_b	Boltzmann Constant	1.38 10^{-23} J.K^{-1}
T	Temperature	K
r_{ENP}	Radius of engineered nanoparticle	m
r_{NCP}	Radius of natural counter particle	m
h	Separation distance	m
$A_{Hamaker(ENP,water,NCP)}$	Hamaker constant between engineered nano- and natural counter particle	10^{-20} J
z	Ion valence	(-)
e	Elemental charge	1.6 10^{-19} C
ζ_{ENP}	Zeta potential of the engineered nanoparticle	mV
ζ_{NCP}	Zeta potential of the natural counter particle	mV
k_{Debye}	Debye length	m

For the Monte Carlo simulation, triangular distributions have been used to express the uncertainty of the attachment efficiencies. The values of 0 and 1 have been selected as minimum and maximum for these distributions, since attachment efficiencies range per definition between 0 and 1. The modes are represented by the attachment efficiencies that have been derived either experimentally or with the DLVO theory. However, they are not inserted as a fixed value, rather in each iteration a mode is derived from its own MC simulation. The parameters used in the application of the DLVO theory are accompanied with a distribution of uncertainty (eq 1-4; SI C Table 2 and 3), while experimentally obtained attachment efficiencies are often presented as a set of values reflecting a range of environmental conditions. Experimentally derived efficiencies are therefore included as a uniform distribution based on the minimal and maximal efficiencies observed within the boundaries of relevant environmental conditions set out in SI table 3.1. The distributions for the modes of DLVO derived efficiencies are the result of a MC simulation performed on eq 1 using the ranges for environmental conditions and ENP properties given in SI D table 2 and 3.

SI D Table 2. Environmental conditions and parameters for simulation of DLVO theory

Parameter	Medium	Distribution type	Range	Default	Reference
Radius of natural colloidal particles(nm)	Freshwater	Pareto	25- 1000	30	Rosse and Loizeau, 2003
	Sediment	Uniform	25 - 225	125	Areepitak & Ren, 2011
	Soil	Triangular	Min= 10; Mode = 60; Max= 200	60	Citeau et al., 2006
Zeta- potential of natural colloids (mV)	Freshwater	Triangular	Min= -9.5; Mode = -8.8; Max= - 7.9	-8.8	Sun et al., 2013
	Sediment	Uniform	Min= -35 ; Max =-21.3	-28	Bunn et al., 2002
	Soil*3	Uniform	Min= -37 Max = +0.62	-19	Citeau et al. 2006 Loux and Savage, 2008
Radius of natural suspended (non-colloidal) particles (µm)	Freshwater	Lognormal	Min =0.05; Mode = 0.5 ; Max= 10	0.5	Buffle and Leppard, 1995
Zeta-potential of suspended particles (mV)	Freshwater	Triangular	Min= -16 Mode = -14 Max = -12	-14	Sun et al., 2013
Debye length (nm^{-1})*1	Freshwater	Custom	Random selection from classification in table SI1	4.8	Hammes et al., 2013
	Sediment*1	Custom	Random selection from classification in table SI1	4.8	Hammes et al., 2013
	Soil*2	Uniform	Min: 5.8 Max: 10.2	5.8	Cornelis et al., 2013
Ion valence*4	Freshwater Sediment Soil	Triangular Min:1 Max: 2	Mode: 1.2 Mode: 1.2 Mode: 1.6	1.2 1.2 1.6	Keller et al., 2010 Keller et al., 2010 Keller et al., 2010

*1 Assumed to be the same as in freshwater above the sediment compartment

*2 Calculated as a function of ionic strength

*3 Calculated as a function of electrophoretic mobility

*4 Calculated from mono : divalent ion ratio

SI D Table 3. ENP property parameters for simulation of DLVO theory

Parameter		Range Distribution	Nano-CeO_2	Nano-TiO_2	Nano-ZnO	Refs.
Hamaker constant (10^{-20}J)	(ENP, water, ENP)	Uniform	Default: 5.57 Range 5.57*1	Default:4.75 Range: 2.5 -7	Default: 2.07 Range: 1.89 -2.24	Karimian, 2007; Loux and Savage, 2008
	(ENP, water,NCP*2)*3	Uniform	Default: 1.96 Range: 1.96	Default: 1.75 Range: 1.3 – 2.2	Default:1.69 Range: 1.14 – 1.24	Lefevre and Jolivet, 2009; Bergstrom, 1997
Zeta-potential (mV)	Fresh water	Uniform (min; max)	Default:-25.5 Range: -34.7; -16.4	Default: -26.2 Range: -34.8 ; -18.0	Default: -27.9 Range: -32.2; -23.6	Keller et al., 2010
	Sediment*3	Uniform (min; max)	Default:-25.5 Range: -34.7; -16.4	Default:-26.2 Range: -34.8; -18.0	Default:-27.9 Range: -32.2; -23.6	Keller et al., 2010
	Soil	Triangular	Default: -15.2 Range -15.2 ± 0.73	Default: -16.1 Range -16.1 ± 0.44	Default: -17.6 Range -17.6 ± 0.44	Keller et al., 2010

*1 No other values reported in literature were found.

*2 The Hamaker constant of SiO_2 particles represents that of natural counter particles (NCPs)

*3 Derived from Hamaker combining relation (CR) method (Eq 5-7) [Lefevre and Jolivet, 2009], with

$A_{NCP} = A_{SiO_2} = 7.59\ 10^{-20}$ J [Bergstrom, 1997] and $A_{water} = 3.7\ 10^{-20}$ J [Israelachvilli, 1992].

*4 Zeta-potential is assumed to be the same as in fresh water

$$A_{ENP,water,ENP} = \left(\sqrt{A_{ENP}} - \sqrt{A_{water}}\right)^2$$

Eq 5Hamaker constant (*J*) for ENPs in water

$$A_{ENP} = A_{ENP,water,ENP} + 2\sqrt{A_{ENP,water,ENP}}\sqrt{A_{water}} + A_{water}$$

Eq 6 Hamaker constant (*J*) for ENPs in vacuum

$$A_{ENP,water,NCP} = \left(\sqrt{A_{ENP}} - \sqrt{A_{water}}\right)\left(\sqrt{A_{NCP}} - \sqrt{A_{water}}\right)$$

Eq 7 Hamaker constant (*J*) for ENP in interaction with natural counter particle

SI D Table 4. Attachment efficiencies between nano-TiO_2, -ZnO, - CeO_2 and natural particles in different environmental media.

ENP	Natural counter particle	Default	Attachment efficiency Range	Reference
Nano-CeO_2	NC in fresh water systems	0.925	0.85 – 1	Velzeboer et al., 2014; Quik 2013
	SPM in fresh water systems	0.98	0.96 – 1	Velzeboer et al., 2014; Quik 2013
	NCs in soil pore water	0.35	$1\ 10^{-6}$ – 1	DLVO calculated
	Solid grain in soil	0.05	0.01 -0.1	Li et al, 2011
	NCs in sediment pore water	$6.5\ 10^{-5}$	$5\ 10^{-14}$ – 0.7	DLVO calculated
	Solid grain in sediments	0.05	0.01 -0.1	Li et al.,2011
Nano-TiO_2	NC in fresh water systems	0.67	$4\ 10^{-2}$ – 1	DLVO calculated
	SPM in fresh water systems	0.42	$3\ 10^{-7}$ -1	DLVO calculated
	NCs in soil pore water	0.23	$5\ 10^{-7}$-1	DLVO calculated
	Solid grain in soil	0.5	$2.69\ 10^{-3}$ – 1	Godinez and Darnault, 2011; Godinez et al., 2013, Petosa et al., 2012
	NCs in sediment pore water	1.7 10-5	$9\ 10^{-14}$- 0.6	DLVO calculated
	Solid grain in sediments	0.5	$1.4\ 10^{-4}$ – 1	Godinez and Darnault, 2011; Godinez et al., 2013, Petosa et al., 2012
Nano- ZnO	NC in fresh water systems	0.62	$2\ 10^{-2}$ – 1	DLVO calculated
	SPM in fresh water systems	0.26	$3\ 10^{-8}$ -1	DLVO calculated
	NCs in soil pore water	0.15	$3\ 10^{-9}$- 1	DLVO calculated
	Solid grain in soil	0.5	$2.4\ 10^{-6}$ – 1	Jones and Su, 2014; Petosa 2012
	NCs in sediment pore water	$3.6\ 10^{-6}$	$3\ 10^{-16}$ – 0.4	DLVO calculated
	Solid grain in sediments	0.5	$2.4\ 10^{-6}$ – 1	Jones and Su, 2014; Petosa 2012

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SI Chapter E: Data Collection And Treatment Natural Variability Of The Environmental System

The system dimensions and advective mass flows of the default SimpleBox(4nano) are according to the environmental exposure estimation guidelines of REACH (SI B Table 1). Data to characterize the natural variability in such an environmental system has been collected from (a) earlier parameter uncertainty analyses on SimpleBox (b) other model studies on the environmental fate of nanoparticles and (c) experimental, model and literature review studies on the natural variability in environmental materials, conditions and flows.

SI E Table 1 REACH standardized model parameters for environmental exposure estimation on a regional scale [ECHA, 2012] relevant for SimpleBox4nano.

Parameter	Value in REACH regional model
Area of the regional system	$4\ 10^4$ km^2
Area fraction of water	0.03
Area fraction soil	0.97
Mixing depth of soil	5 cm
Atmospheric mixing height	1000 m
Depth of water	3 m
Depth of sediment	3 cm
Average annual precipitation	700 mm.yr^{-1}
Wind speed	3 m.s^{-1}
Residence time of air	0.7 d
Residence time of water	40 d
Fraction of rainwater infiltrating soil	0.25
Fraction of rainwater running off soil	0.25

SI E Table 2. Model parameter distribution reflecting the natural variability for system dimensions, advective flows, and natural particles in the compartments atmosphere, fresh water, soil, and sediment. The shape of the distribution are lognormal (L), triangular (T), uniform (U), Pareto (P), and Weibull (W).

Parameter name	Distri-bution shape	Default, Mean (L), Mode (T), Value (C), Scale (W)	Min (T,P) Location (L,W)	Max (T,P) Shape (W) St. Dev. (L)	Reference
System temperature ˚C	T	10	-5	30	Bakker et al., 2003
N nucleation aerosols (#.cm^{-3})	L	1.4 10^3	-3.2 10^3	4.0 10^2	Neususs et al., 2002*[1]
Diameter nucleation aerosols (µm)	L	2 10^{-2}	(-)	1.6 10^{-1}	Jaenicke et al., 1993
Density nucleation aerosols (kg.m^{-3})	T	1.3 10^3	5.0 10^2	1.5 10^3	Kannosto et al., 2008
N accumulation aerosols(#.cm^{-3})	L	3.6 10^3	1.2 10^3	4.0 10^3	Neususs et al., 2002
Diameter accumulation aerosols(µm)	L	1.2 10^{-1}	(-)	2.2 10^{-1}	Jaenicke et al., 1993
Density accumulation	T	1.5 10^3	1.1 10^3	2.0 10^3	Kannosto et al., 2008

aerosols (kg.m^{-3})					
N coarse aerosols (#.cm^{-3})	L	2.1	-1.3 10^{-1}	3.4	Neususs et al., 2002
Diameter coarse aerosols (µm)	L	1.8	(-)	0.43	Jaenicke et al., 1993
Density coarse aerosols*^{1} (kg.m^{-3})	T	1.6 10^{3}	1.6 10^{3}	1.9 10^{3}	Neususs et al., 2002
Friction velocity (m.s^{-1})	T	2.5 10^{-1}	1.1 10^{-1}	4.0 10^{-1}	Nho-Kim et al., 2004
Viscous : Total Drag ratio	U	0.27	¼	1/3	Slinn, 1982
Fraction of interception by large collectors (%)	U	5.5	1	10	Slinn, 1982
Small vegetation hair width (µm)	U	5	0	10	Slinn, 1982
Large vegetation collector radius (mm)	U	0.75	0.5	1	Slinn, 1982
Rain dry air ratio	U	(-)	1 10^{-7}	3 10^{-7}	Franco and Trapp, 2010
Wind speed (m.s^{-}	T	5.0	1.7	14	Bakker et

^{1})					al., 2003
Rainrate (mm.d-1)	T	2.0	2 10^{-2}	6.6	Bakker et al., 2003
NC number concentration in fresh water (#.m^{-3})	T	1.7 10^{14}	4.8 10^{13}	4 10^{14}	Gallego-Urrea et al., 2010
NC size in freshwater (nm)	P	(-) Default: 60	50	2000	Rosse and Loizeau, 2003
NC density in fresh water (kg.m^{-3})	T	1.3 10^{3}	1.1 10^{3}	2.5 10^{3}	Velzeboer et al., 2014
SP number concentration in fresh water (#.m^{-3})	U	3.6 10^{10}	9.2 10^{9}	6.3 10^{10}	Praetorius et al., 2012
SP size in freshwater (µm)	L	5	(-)	0.6	Praetorius et al., 2012
SP density in fresh water (kg.m^{-3})	U	1.8 10^{3}	1.1 10^{3}	2.5 10^{3}	Praetorius et al., 2012
Water depth (m)	W	3	2	15	Bakker et al., 2003
Water Flow (m^{3}.s^{-}	L	2.3 10^{3}		8.9 10^{2}	Bakker et

^{1})					al., 2003
Fresh water shear stress (s^{-1})	U	5	0	10	Praetorius et al., 2012
NC number concentration in soil pore water (#.m^{-3})	T	7 10^{13}	3 10^{12}	4 10^{14}	Rani et al., 2011
NC size in soil pore water (nm)	T	1.2 10^{2}	20	4 10^{2}	Citeau et al, 2006
NC density in soil pore water (kg.m^{-3})	U	(-)	2000	2700	Citeau et al, 2006
Soil grain radius (µm)	T	1.3 10^{2}	62	2.9 10^{2}	Cornelis et al., 2013
Soil pore water filtration velocity (m.s^{-1})	T	7 10^{-6}	1 10^{-4}	2 10^{-3}	Schwartz et al., 2000; Tufenkji andElimelech, 2004
Soil Erosion (mm.y-1)	T	3 10^{-2}	7.5 10^{-4*2}	6 10^{-2}	Bakker et al., 2003
FR rainwater run-off (-)	T	0.25	6.3 10^{-3*2}	0.5	Bakker et al., 2003
FR rainwater infiltration (-)	T	0.25	6.3 10^{-3*2}	0.5	Bakker et al., 2003

Soil porosity	T	0.20	3 10^{-3}	0.67	Bakker et al., 2003
Density of soil solids (kg.m^{-3})	T	2.5 10^{3}	2.0 10^{3}	3.0 10^{3}	Bakker et al., 2003
Sediment grain radius(µm)	T	1.3 10^{2}	6	2.0 10^{2}	Velzeboer et al., 2014; Jones and Su, 2012
Sediment water filtration velocity (m.s^{-1})*2	U	(-) Default: 5 10^{-7}	10^{-9}	10^{-6}	Higashino et al., 2009
Sediment depth (m)	T	3 10^{-2}	1 10^{-2}	0.1	Bakker et al., 2003
Sediment porosity	T	0.8	0.5	0.99	Bakker et al., 2003
Sediment resuspension (m.h^{-1})	T	1.1 10^{-8}	0	2.3 10^{-8*3}	Praetoriues et al., 2012
Sediment burial rate (m.y^{-1})	T	2.7 10^{-3}	1 10^{-3}	5 10^{-2}	Bakker et al., 2003; Koelmans et al., 2009

*1 Calculated from raw data of Neususs et al., 2002

*2 Minimal value assumed to be 2.5% of median

*3 Maximum value assumed to be 2 times larger than median

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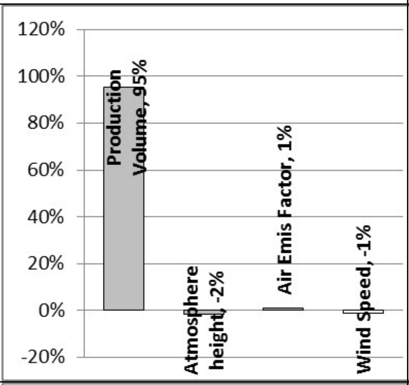
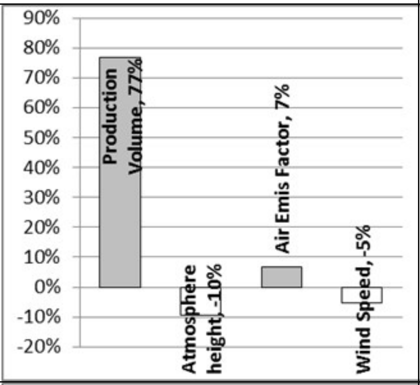
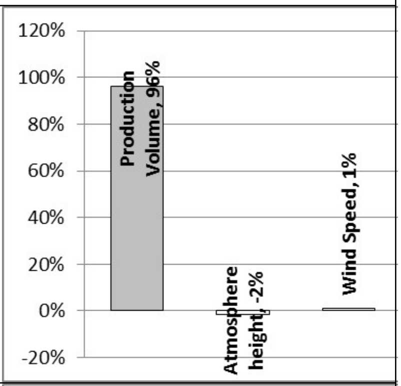
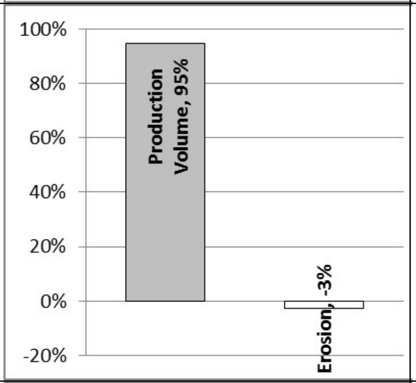
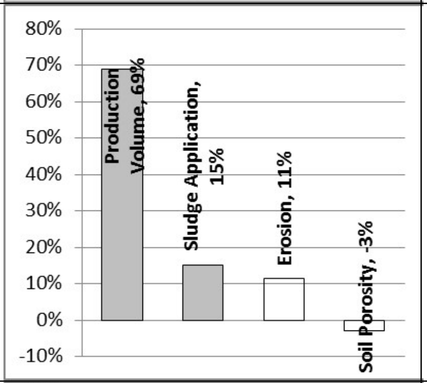
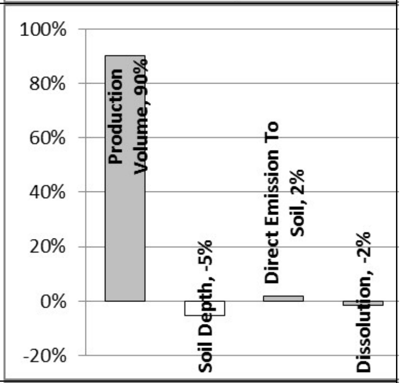
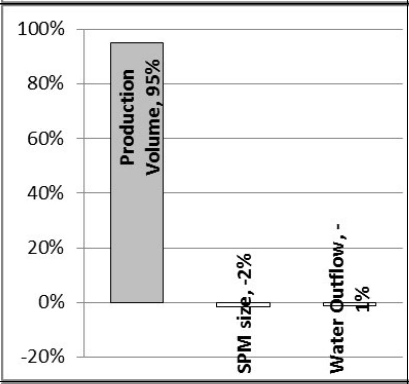
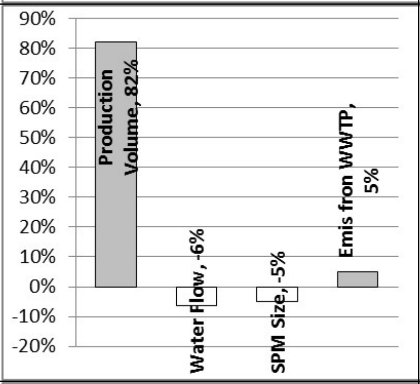
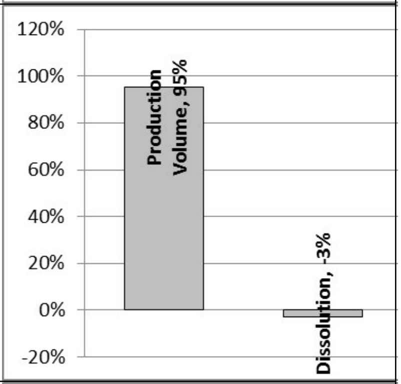
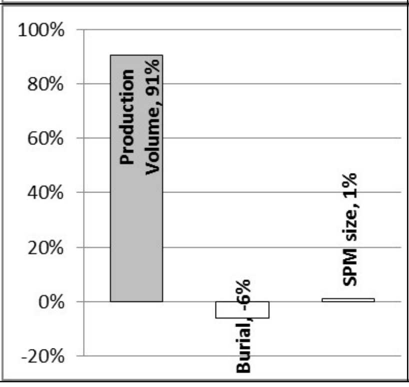
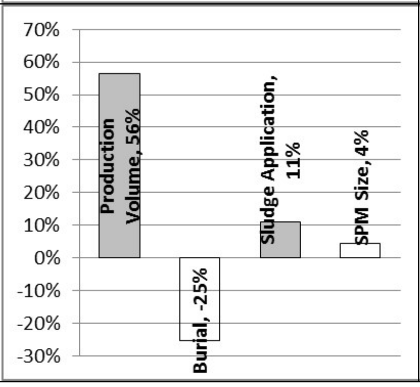
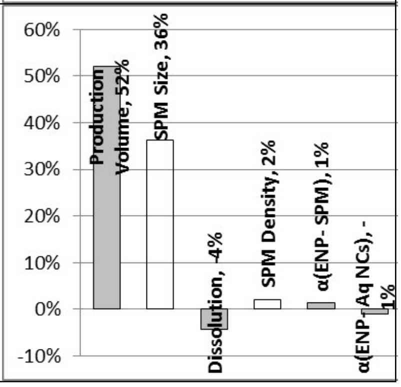
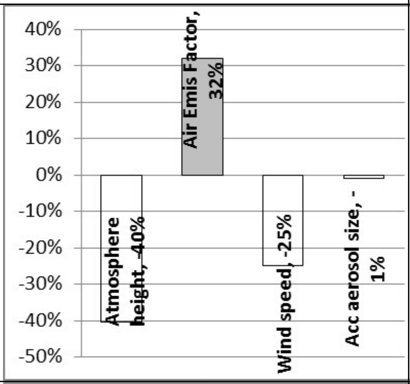
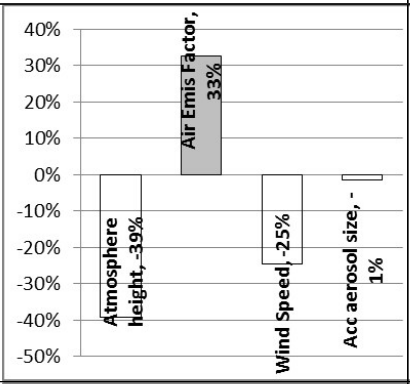
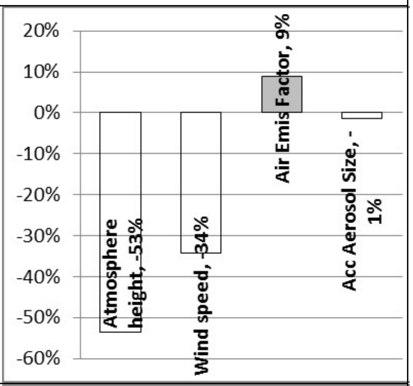
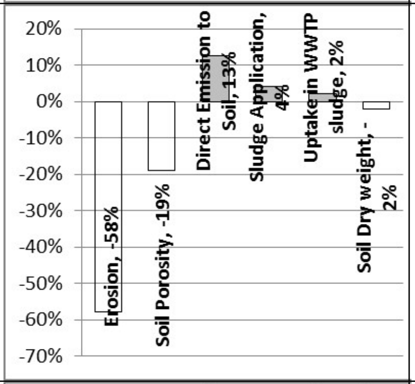
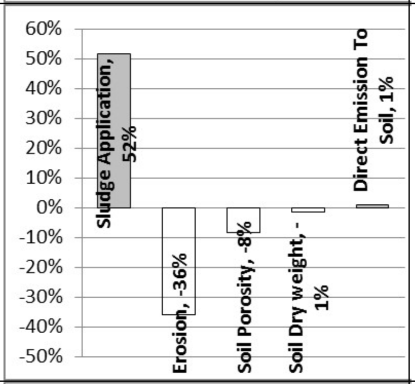
SI Chapter F: Spearman Rank Analysis Results

SI F Table 1. Spearman Rank coefficients for the predicted environmental concentrations of nano-CeO2, -TiO2, and –ZnO.

	Nano-CeO$_2$	Nano-TiO$_2$	Nano-ZnO
Atmosphere (g.m^{-3})			
Soil (g.kg^{-1})			
Water (g.m^{-3})			
Sediment (g.kg^{-1})			

Grey bars represent uncertainty in input parameters, white bars variability in model parameters.

SI F Table 2. Spearman Rank coefficients for the environmental distribution ((PEC).($t_{produced}$.y^{-1})$^{-1}$) of nano-CeO2, -TiO2, and -ZnO

<table>
<tr><th></th><th>Nano-CeO_2</th><th>Nano-TiO_2</th><th>Nano-ZnO</th></tr>
<tr><td>Atmosphere (g.m^{-3}).(tproduced.y^{-1})$^{-1}$</td>
<td>
</td>
<td>
</td>
<td>
</td></tr>
<tr><td>Soil (g.kg^{-1}).($t_{produced}$.y^{-1})$^{-1}$</td>
<td>
</td>
<td>
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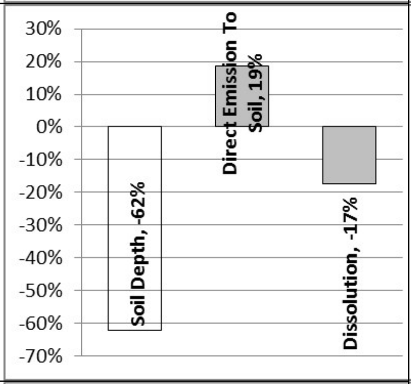
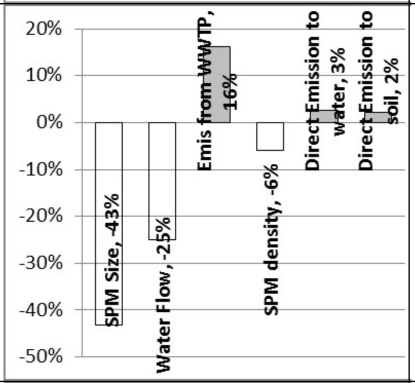
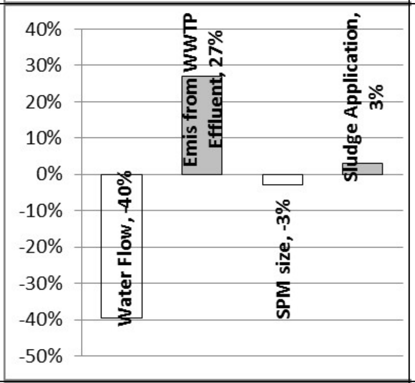
<td>
</td></tr>
<tr><td>Water (g.m^{-3})($t_{produced}$.y^{-1})$^{-1}$</td>
<td>
</td>
<td>
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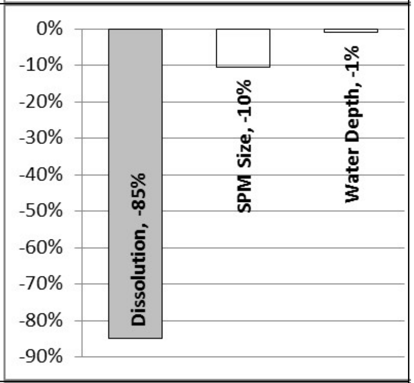
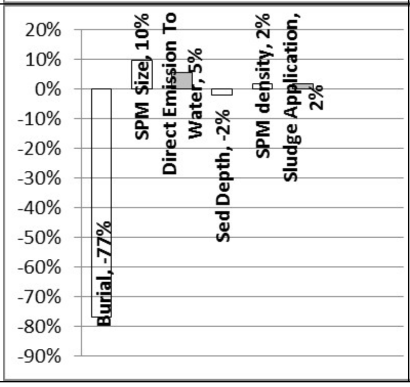
<td>
</td></tr>
<tr><td>Sediment (g.kg^{-1}).($t_{produced}$.y^{-1})$^{-1}$</td>
<td>
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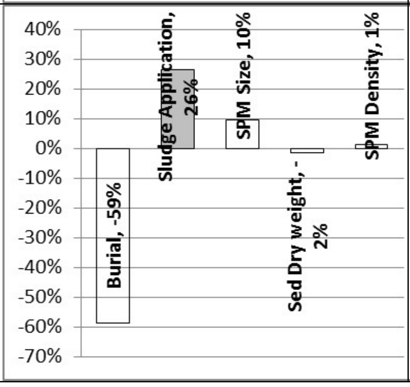
<td>
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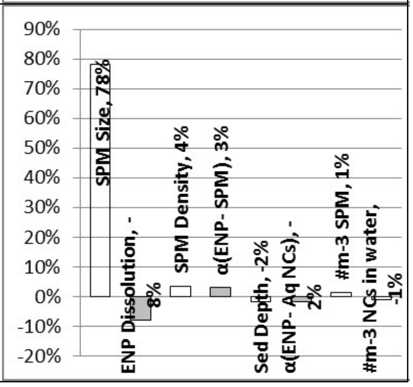
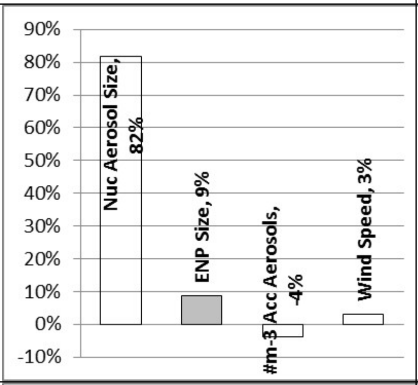
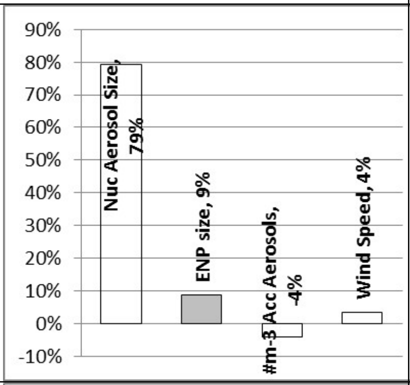
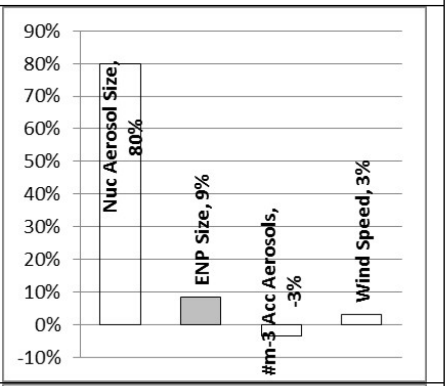
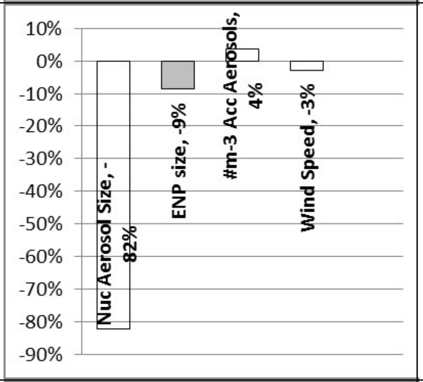
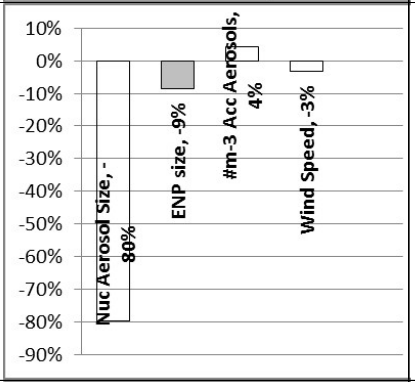
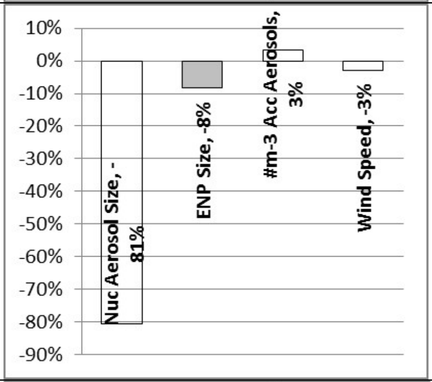
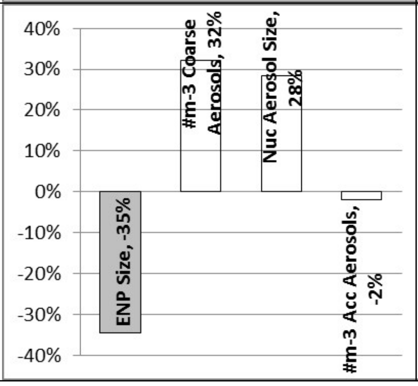
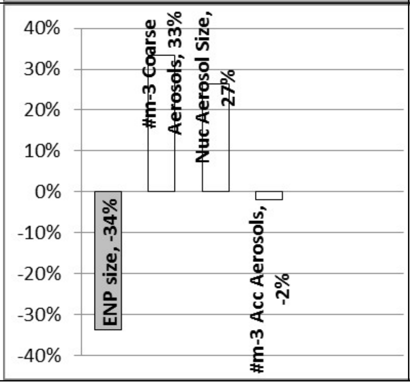
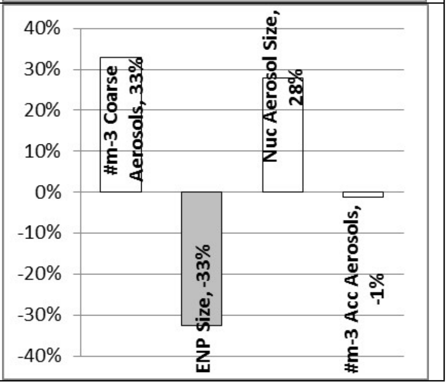
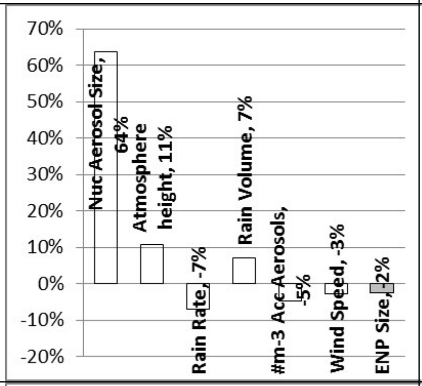
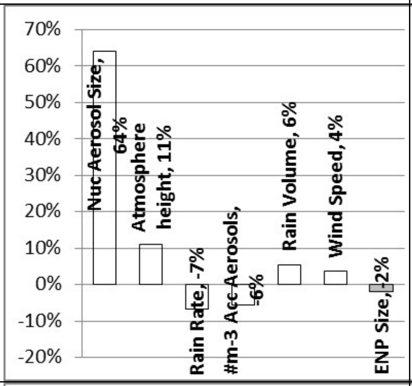
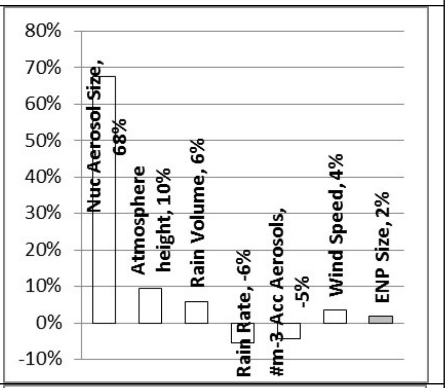
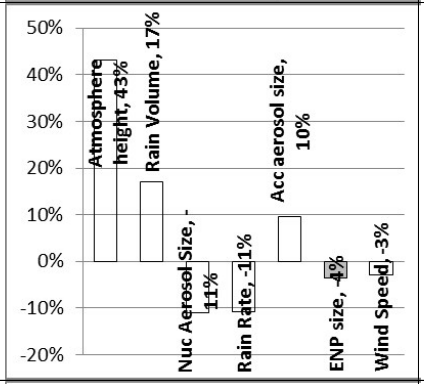
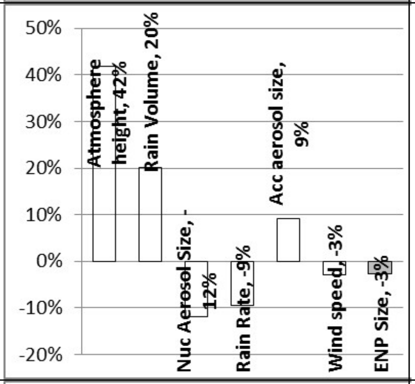
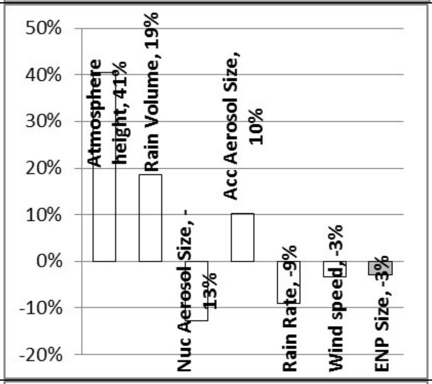
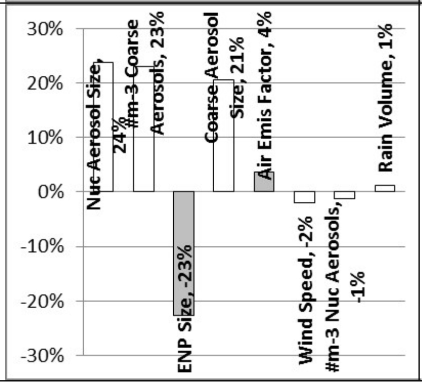
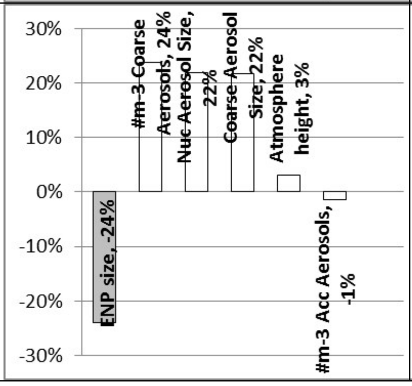
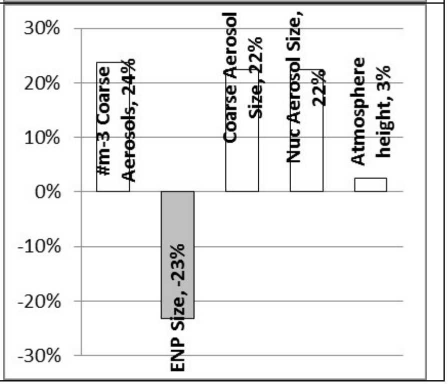
<td>
</td></tr>
</table>

SI F Table 3. Spearman Rank coefficients for the species distribution pattern of nano-CeO2, -TiO2, and -ZnO in the atmosphere ($g_{species}.g_{totalincompartment}^{-1}$)

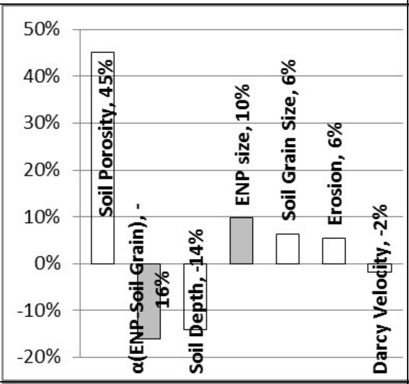
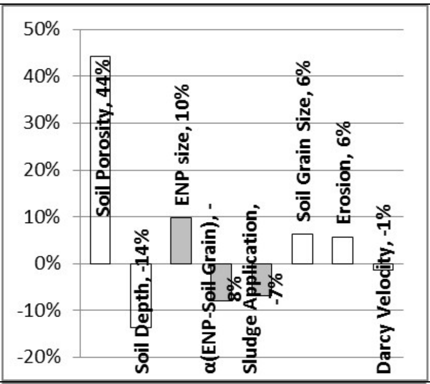
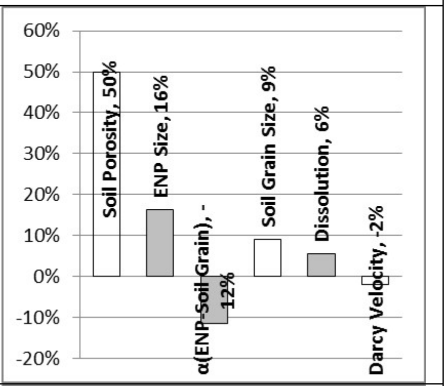
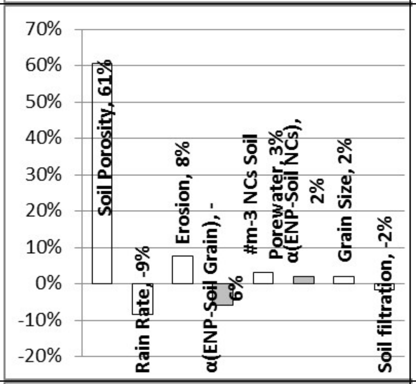
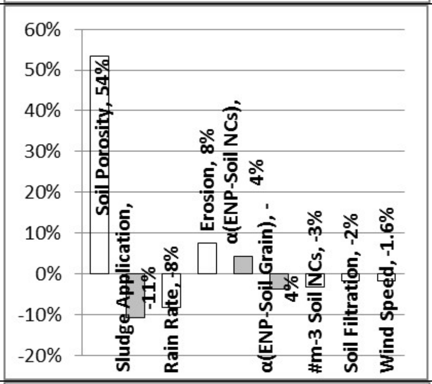
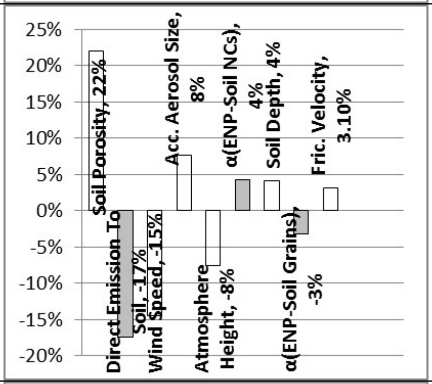
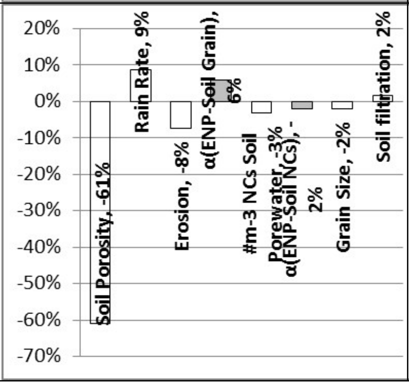
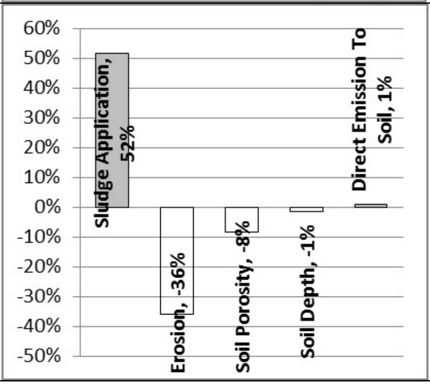
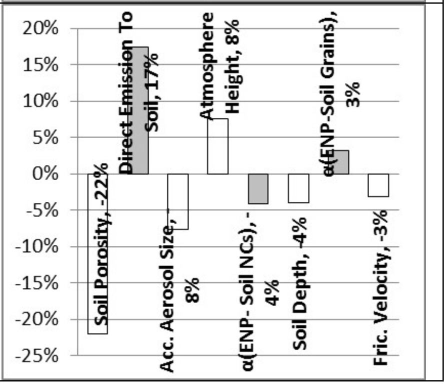
	Nano-CeO_2	Nano-TiO_2	Nano-ZnO
Free in dry air			
Aggregated in dry air			
Attached in dry air			

Grey bars represent uncertainty in input parameters, white bars variability in model parameters.

SI F Table 3. Spearman Rank coefficients for the species distribution pattern of nano-CeO2, -TiO2, and -ZnO in the atmosphere ($g_{species}.g_{totalincompartment}^{-1}$) continued

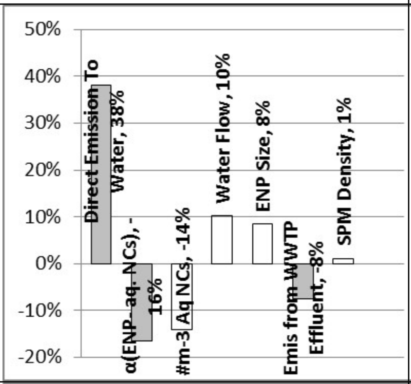
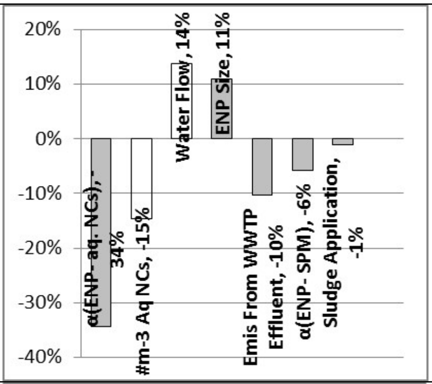
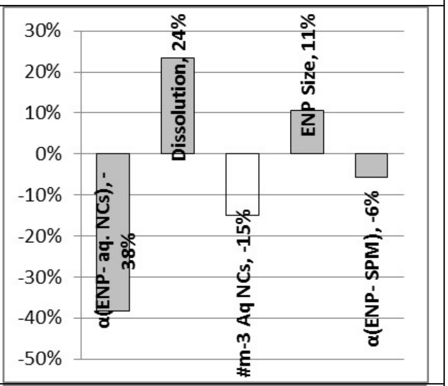
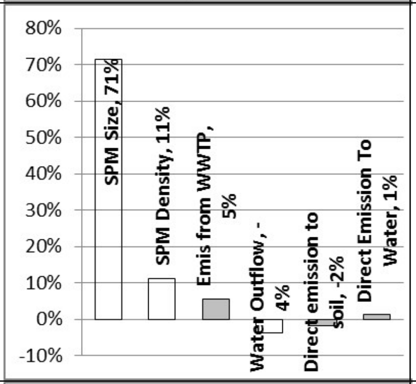
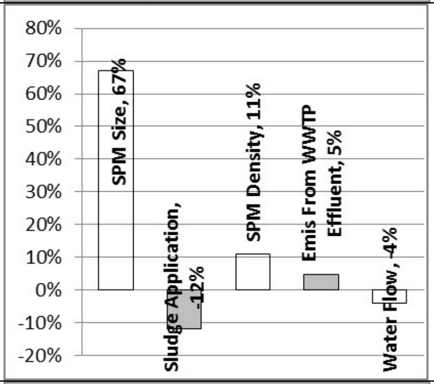
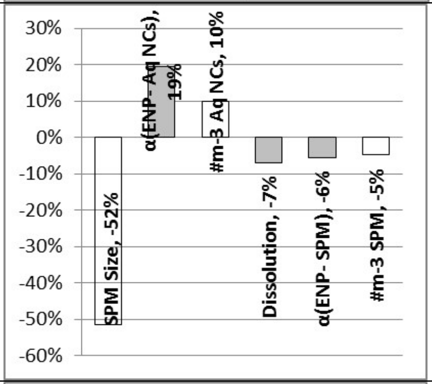
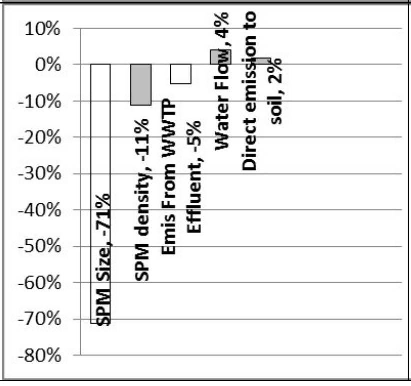
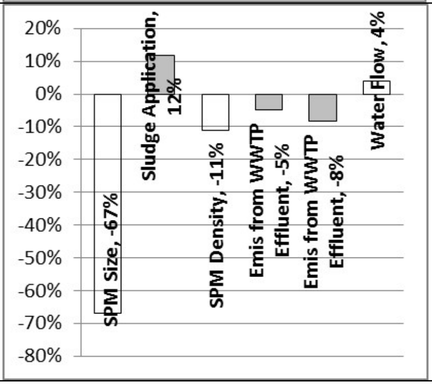
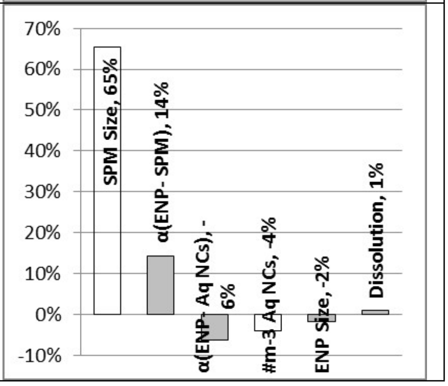
	Nano-CeO_2	Nano-TiO_2	Nano-ZnO
Free in raindrop			
Aggregated in raindrop			
Attached in raindrop			

SI F Table 4. Spearman Rank coefficients for the species distribution pattern of nano-CeO2, -TiO2, and -ZnO in soil

	Nano-CeO$_2$	Nano-TiO$_2$	Nano-ZnO
Free in Soil			
Aggregated in Soil			
Attached in Soil			

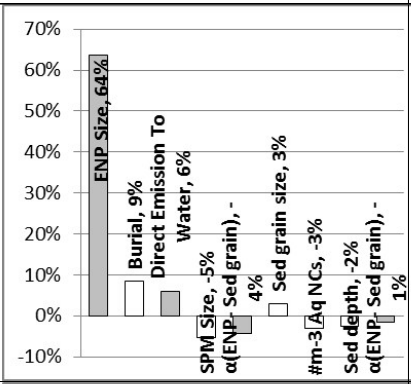
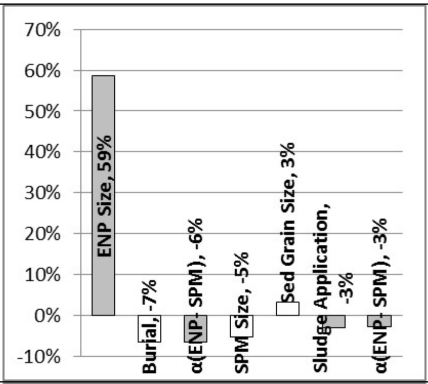
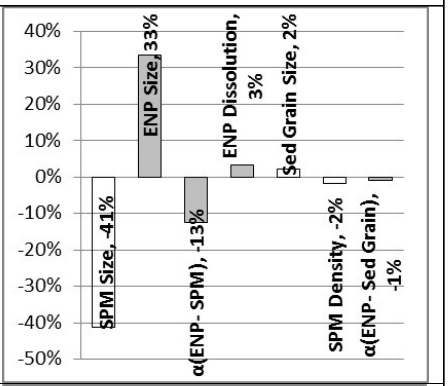
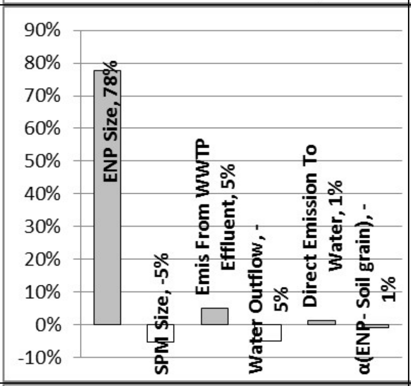
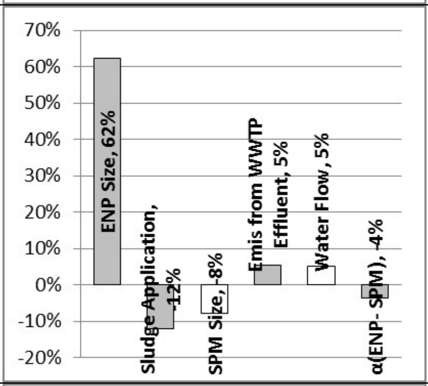
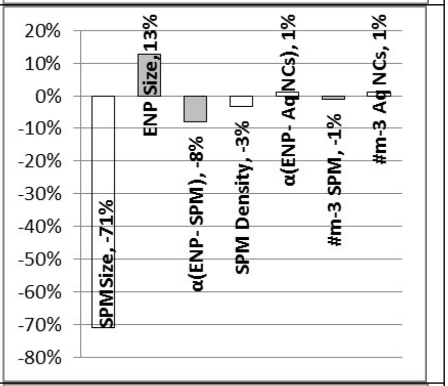
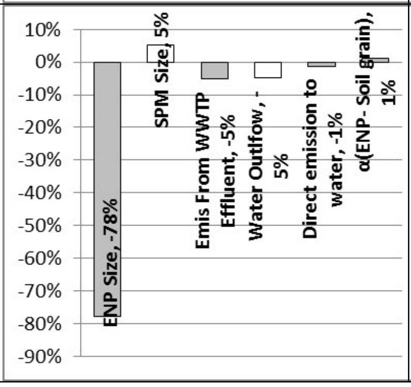
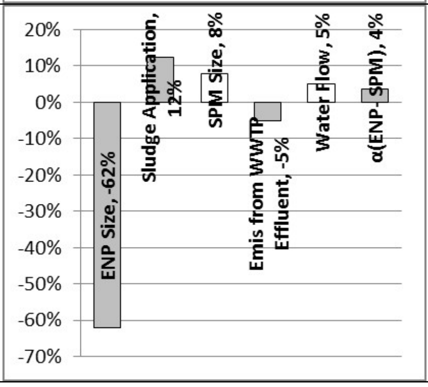
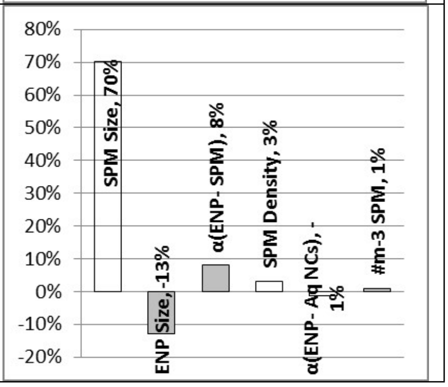
Grey bars represent uncertainty in input parameters, white bars variability in model parameters.

SI F Table 5. Spearman Rank coefficients for the species distribution pattern of nano-CeO2, -TiO2, and -ZnO in water

	Nano-CeO$_2$	Nano-TiO$_2$	Nano-ZnO
Free in Water			
Aggregated in Water			
Attached in Water			

Grey bars represent uncertainty in input parameters, white bars variability in model parameters.

SI F Table 6. Spearman Rank coefficients for the species distribution pattern of nano-CeO2, -TiO2, and -ZnO in sediments

	Nano-CeO_2	Nano-TiO_2	Nano-ZnO
Free in Sediments			
Aggregated in Sediments			
Attached in Sediments			

The highest absolute values in the Spearman Rank correlation coefficients represent the largest sources of uncertainty or variability. A negative coefficient means that an increase of the respective parameter leads to a decrease of the dependent ENPs' environmental or species distribution, the opposite applies for a positive coefficient.

SI Chapter G: Comparison Simulated Environmental Fate SimpleBox4nano With Fate Patterns Reported In Literature

SI G Table 1. Comparison Simulated Environmental Fate SimpleBox4nano With Fate Patterns Reported In Literature

ENPs	Environmental Fate of ENPs according to literature	Expected Environmental Pattern of ENPs	Comparison with MC results of SB4N
In the atmosphere	-Little emission (1,2,3) -Effective removal through deposition, coagulation with natural aerosol particles (2,4,5) -No diffusive transport from other compartments into the atmosphere (2,6,7)	-Relatively low concentrations	-Total concentrations in the atmosphere are the lowest of all environmental compartments
In soil	-High emission scenarios for soils treated sewage sludge containing ENPs (8). -Accumulation expected for ENPs attaching to soil grains (9,10,11). -Attached ENPs are limited in their mobility (12) so that removal by leaching to deeper groundwater is unlikely (2).	-High concentrations of ENP attached species	-The attached ENP species are significantly the largest fraction in soil for all three types of ENP investigated. -Accumulation ENPs through attachment with solid grains (SI 5) -The majority of free ENPs attaches to the solid grains of soil “within minutes”, whereas removal of attached ENPs by dissolution takes “months” and by erosion alone even “centuries”.
In water	-Relatively high emission with respect to the size of the compartment (1,7). -The dominant removal mechanism is through hetero-aggregation and attachment to natural particles settling to the bottom (13,14,15). -ENPs that are not associated with natural particles can still settle	-High uncertainty expected -The interaction between ENPs and natural particles is complex and difficult to predict (17) - The interaction between ENPs and natural particles is dominant for their aquatic fate (2,13,14,15,16).	-Total concentrations in water are the highest of all environmental compartments. -ENPs aggregated with natural colloids are significantly the dominant species of occurrence (figure 3). -Uncertainty is not large compared to other compartments, but the parameters simulating the interaction between ENPs and natural particles dominate the

	on their own (16), but are more prone to remain in the water as a non-settling fraction (13,14,15).	-High total concentrations can be expected since there is relatively high emission into a relatively small compartment (1,2).	uncertainty for all aquatic ENP concentrations.
In sediment	-The aquatic fate of ENPs is also determinant for sediment concentrations (15,16). -The dominant influx of ENPs is through sedimentation of ENPs associated with natural particles (13,15). -Settling natural particles also bury the top layer of the sediment, so that high influx of ENPs also yields effective removal by burial (18). -Concentrations are expected to differ between the top and deeper layers of sediment -In the top layer there is removal through burial (18) and resuspension (19) -The deeper layers of sediment are regarded as the final sink for ENPs (2,10,20,21).	-ENP concentrations in the top layer of sediment are strongly related to the aquatic concentrations (12). -Sediment concentrations of free ENPs will be very low, because they are prone to reside in the water compartment (13,14,15). -High concentrations are especially expected in the deeper layers of sediment, because of accumulation (2,10,20,21).	- SB4N only considers the top layer of the sediment compartment, which is considered to be the secondary compartment of water. -In contrast to the water compartment, the aggregated species is not dominant compared to the attached species (figure 3). -The ENPs attached to the larger suspended particles settle more effectively than ENPs aggregated with the smaller colloid particles (SI G Table 3). -Only a very small amount of free ENPs settle to the sediment compartment through self-sedimentation. -The attached ENPs species in sediment are mainly a result of ENP attachment to suspended particles in the water column (SI F Table 4).
Associated with natural particles	-Only a small proportion of ENPs can persist in their pristine (free) state Under natural conditions(22,23,24). -These proportions have not been quantified before (23) as existing models oversimplify or disregard transformation and (hetero-)aggregation processes at all (22,23,24), -Current measurement techniques are not able to detect ENPs attached to and aggregated with natural particles (24).	-Free (pristine) ENP represent a small fraction of the total concentrations of ENPs in the environment (22,23,24).	-For all three types of ENP investigated the free ENPs are significantly the smallest fraction in all environmental compartments except for the atmosphere. -For all the other compartments the fraction of free ENPs are most-likely to be <1% and never larger than 5%.

Dissolved	-Dissolution is a removal process for ENPs (6,7). -Nano-TiO_2 and -CeO_2 are found to be practically insoluble (7,25,26,27) - Nano-ZnO can dissolve under natural conditions (7,28). -Even poorly soluble solids can and will dissolve to some extent eventually given the large volumes of water in the environment (6) -Chemical reactions such as oxidation and / or sulfidication also lead to dissolution of ENPs (6,29).	-Concentrations of highly soluble ENPs are most effectively reduced by dissolution (2).	-Nano-ZnO is simulated as the most soluble of the three ENPs investigated (2), but also with the highest emission distribution to water (1). -The reduction of nano-ZnO by dissolution can be observed from MC results: in water and soil the concentration ratios between n-ZnO with n-CeO_2 and n-TiO_2 are smaller than the respective emission ratios. -The reduction is strongest for the aggregated and attached species, because then dissolution works as a two-fold mechanism (1) aggregated and attached ENPs dissolve themselves and (2) less free ENPs will attach or aggregate with natural particles as they are already dissolved.

(1) Keller et al., 2013, (2) Garner and Keller, 2014, (3) Keller and Lazareva, 2014, (4) Tiwari and Marr, 2010, (5) Kumar et al., (2010), (6) Meesters et al., 2013, (7) Quik et al., 2011), (8) Nowack et al., 2012, (9) Lin et al., 2010, (10) Batley et al, 2013, (11) Cornelis et al., 2013, (12) Brant et al., 2005, (13) Quik et al., 2012, (14) Quik et al., 2014, (15) Velzeboer et al., 2014, (16) Praetorius et al., 2012, (17) Petosa et al., 2010, (18) Koelmans et al., 2009, (19) Pakarinen et al., 2014, (20) Dale et al., 2013, (21) Liu and Cohen, 2014, (22) Isaacson et al., 2009, (23) Hendren et al., 2013, (24) Gottschalk et al., 2013), (25) Schmidt and Vogelsberger, 2009, (26) Simon-Deckers et al., 2009, (27) Van Hoecke et al. 2009, (28) David et al., 2012, (29) Praetorius e al., 2013.

SI G Table 2. Accumulation of ENPs in soil through attachment with soil grains simulated with SimpleBox4nano

	Nano-CeO$_2$ med (95%CI)	Nano-TiO$_2$ med (95%CI)	Nano-ZnO med (95%CI)
Dry deposition of ENPs attached to coarse aerosols $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	4.1 10^{-10} (7.1 10^{-13} – 1.6 10^{-8})	2.7 10^{-10} (6.4 10^{-13} - 1.0 10^{-8})	1.1 10^{-9} (1.8 10^{-12} -3.7 10^{-8})
Wet deposition of ENPs attached to coarse aerosols $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	3.7 10^{-10} (4.6 10^{-13} – 2.8 10^{-8})	2.4 10^{-10} (4.1 10^{-13} -1.8 10^{-8})	9.5 10^{-10} (1.4 10^{-12} -6.8 10^{-8})
Total deposition of ENPs attached to coarse aerosols $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	9.9 10^{-10} (1.6 10^{-12} – 4.3 10^{-8})	6.6 10^{-10} (1.5 10^{-12} - 2.8 10^{-8})	2.6 10^{-9} (4.6 10^{-12} -9.6 10^{-8})
Attachment of free ENPs in soil pore water to soil grains $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	1.5 10^{-4} (6.5 10^{-5} -2.3 10^{-4})	1.3 10^{-4} (6.5 10^{-5} -2.1 10^{-4})	1.1 10^{-4} (3.5 10^{-5} -1.8 10^{-4})
Attachment rate of free ENPs in soil (s^{-1})	4.7 10^{-2} (1.9 10^{-3} – 1.7)	7.4 10^{-2} (3.7 10^{-3} -2.3)	7.4 10^{-2} (3.6 10^{-3} -2.5)
Dissolution of ENPs in soil (s^{-1})	0	0	1.0 10^{-6} (4.0 10^{-7} -1.6 $^{10-6}$)
Erosion rate of ENPs in soil (s^{-1})	4.1 10^{-12} (7.4 10^{-13} -3.0 10^{-11})	4.1 10^{-12} (7.5 10^{-13} -3.0 10^{-11})	4.1 10^{-12} (7.3 10^{-13} -3.1 10^{-11})
Total removal rate of ENPs attached to grains in soil (s^{-1})	1.8 10^{-7} (8.9 10^{-9} – 3.6 10^{-7})	1.9 10^{-7} (8.9 10^{-9} -3.6 10^{-7})	1.0 10^{-6} (4.1 10-7 -1.6 10-6)

SI G Table 3 Mass flows of free, aggregated and attached ENPs within and into sediment simulated with SimpleBox4nano

	Nano-CeO2 med (95%CI)	Nano-TiO2 med (95%CI)	Nano-ZnO med (95%CI)
Settling rate of free ENPs ($m.s^{-1}$)	8.9 10^{-9} (3.8 10^{-11} -3.2 10^{-8})	4.6 10^{-9} (2.1 10^{-11} - 1.7 10^{-8})	5.9 10^{-9} (3.3 10^{-11} -2.4 10^{-8})
Settling rate of agg ENPs ($m.s^{-1}$)	6.8 10^{-9} (4.1 10^{-10} -3.0 10^{-8})	3.9 10^{-9} (3.9 10^{-10} -1.5 10^{-8})	4.7 10^{-9} (4.1 10^{-10} -2.2 10^{-8})
Settling rate of att ENPs ($m.s^{-1}$)	1.8 10^{-5} (5.2 10^{-7} - 5.8 10^{-4})	1.8 10^{-5} (5.1 10^{-7} - 6.0 10^{-4})	1.9 10^{-5} (4.8 10^{-7} -6.2 10^{-4})
Mass flow settling free ENPs $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	1.3 10^{-11} (1.2 10^{-14} -2.0 10^{-10})	1.0 10^{-10} (8.8 10^{-14} -1.2 10^{-9})	1.7 10^{-10} (1.710^{-13} -2.3 10^{-9})
Mass flow settling agg ENPs $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	1.8 10^{-7} (8.5 10^{-9} - 1.4 10^{-6})	7.7 10^{-7} (5.4 10^{-8} -4.8 10^{-6})	2.2 10^{-8} (1.2 10^{-9} - 2.2 10^{-7})
Mass flow settling att ENPs $(g_{ENP}.s^{-1})(t_{produced}.y^{-1})^{-1}$	1.6 10^{-4} (3.7 10^{-5} - 2.9 10^{-4})	5.3 10^{-4} (8.6 10^{-5} - 1.2 10^{-3})	1.3 10^{-6} (1.9 10^{-9} -1.6 10^{-4})

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SI Chapter H: Calculation Of Conservative Correction Factors For Default PECs

The MC simulations with SB4N both deliver PECs ($g_{ENP}.m_{air}^{-3}$, $g_{ENP}.m_{water}^{-3}$, $g_{ENP}.kg_{sed\cdot dryweight}^{-1}$ $g_{ENP}.kg_{soil.dryweight}^{-1}$) as single default and probibalistically derived median values with 95% CIs. The conservative correction factors for the default PECs are calculated as the ratio of the 97.5 and 2.5 percentile of the probabilistically derived PECs. Furthermore, the 95% CI of the PECs calculated with the MC simulations include the uncertainty in the estimation of production volumes, whereas legislation in chemical risk assessment is based on registrated production volumes. Hence, correction factors are calculated for free ENPs, “bioavailable” ENPs (i.e. the sum of free and ENPs hetero-aggregated with natural colloids), and the total amount of ENPs in the compartments air, water, sediment and soil. These correction factors are derived for both the scenarios of certain and uncertain production volumes.

SI H Table 1. Calculation Of Conservative Correction Factors For Default PECs for nano-CeO_2

($g_{ENP} \cdot m_{air}^{-3}$, $g_{ENP} \cdot m_{water}^{-3}$, $g_{ENP} \cdot kg_{sed \cdot dryweight}^{-1}$ $g_{ENP} \cdot kg_{soil.dryweight}^{-1}$)

		Inclusive Uncertainty Production Volume				Exclusive Uncertainty Production Volume			
Environmental Exposure	Default PEC	Median	2.5 Percentile	97.5 Percentile	**Assessment Factor**	Median	2.5 Percentile	97.5 Percentile	**Assessment factor**
Free in Air	1E-12	1E-12	1E-15	8E-10	**6E+05**	3E-13	2E-15	3E-12	**2E+03**
Bioavailable in air	2E-12	1E-11	8E-14	4E-09	**5E+04**	2E-12	6E-13	7E-12	**1E+01**
Total in Air	2E-12	1E-11	8E-14	4E-09	**5E+04**	2E-12	6E-13	7E-12	**1E+01**
Free In Water	2E-9	4E-10	1E-12	2E-07	**1E+05**	8E-11	5E-12	5E-10	**1E+02**
Bioavailable in Water	5E-6	8E-06	4E-08	2E-03	**5E+04**	1E-06	4E-07	4E-06	**1E+01**
Total in Water	1E-5	1E-05	7E-08	4E-03	**5E+04**	2E-06	5E-07	6E-06	**1E+01**
Free in Sediment	1E-16	6E-18	4E-22	8E-15	**2E+07**	1E-18	1E-22	6E-17	**4E+05**
Bioavailable In Sediment	9E-10	4E-08	1E-10	3E-05	**3E+05**	8E-09	3E-10	1E-07	**5E+02**
Total in Sediment	5E-7	4E-05	2E-07	1E-02	**7E+04**	6E-06	1E-06	5E-05	**4E+01**
Free In soil	3E-14	4E-14	7E-17	3E-11	**4E+05**	6E-15	1E-16	2E-13	**2E+03**
Bioavailable in soil	2E-11	8E-10	2E-12	4E-07	**2E+05**	1E-10	7E-12	2E-09	**3E+02**
Total In soil	1E-4	5E-04	3E-06	1E-01	**5E+04**	8E-05	2E-05	4E-04	**1E+01**

SI H Table 2. Calculation Of Conservative Correction Factors For Default PECs for nano-TiO_2 ($g_{ENP}.m_{air}^{-3}$, $g_{ENP}.m_{water}^{-3}$, $g_{ENP}.kg_{sed\cdot dryweight}^{-1}$ $g_{ENP}.kg_{soil.dryweight}^{-1}$)

		Inclusive Uncertainty Production Volume				Exclusive Uncertainty Production Volume			
Environmental Exposure	Default PEC	Median	2.5 Percentile	97.5 Percentile	**Assessment Factor**	Median	2.5 Percentile	97.5 Percentile	**Assessment factor**
Free in Air	2E-10	1E-11	7E-14	4E-10	**6E+03**	3E-11	2E-13	3E-10	**1E+03**
Bioavailable in air	3E-10	1E-10	9E-12	1E-09	**1E+02**	3E-10	8E-11	8E-10	**1E+01**
Total in Air	3E-10	1E-10	9E-12	1E-09	**1E+02**	3E-10	8E-11	8E-10	**1E+01**
Free In Water	3E-7	9E-08	3E-09	1E-06	**3E+02**	2E-07	2E-08	1E-06	**7E+01**
Bioavailable in Water	1E-3	9E-04	6E-05	7E-03	**1E+02**	2E-03	5E-04	4E-03	**8E+00**
Total in Water	1E-3	1E-03	8E-05	9E-03	**1E+02**	2E-03	5E-04	4E-03	**8E+00**
Free in Sediment	1E-14	5E-16	5E-20	4E-14	**9E+05**	1E-15	1E-19	5E-14	**4E+05**
Bioavailable In Sediment	3E-5	3E-06	6E-08	7E-05	**1E+03**	5E-06	3E-07	8E-05	**3E+02**
Total in Sediment	3E-2	2E-03	9E-05	3E-02	**3E+02**	4E-03	5E-04	3E-02	**6E+01**
Free In soil	4E-12	3E-13	4E-15	1E-11	**4E+03**	6E-13	1E-14	2E-11	**1E+03**
Bioavailable in soil	4E-9	6E-09	2E-10	2E-07	**1E+03**	1E-08	8E-10	3E-07	**3E+02**
Total In soil	7E-2	2E-02	1E-03	3E-01	**2E+02**	5E-02	9E-03	2E-01	**3E+01**

SI H Table 3. Calculation Of Conservative Correction Factors For Default PECs for nano-ZnO ($g_{ENP}.m_{air}^{-3}$, $g_{ENP}.m_{water}^{-3}$, $g_{ENP}.kg_{sed\cdot dryweight}^{-1}$ $g_{ENP}.kg_{soil.dryweight}^{-1}$)

		Inclusive Uncertainty Production Volume				Exclusive Uncertainty Production Volume			
Environmental Exposure	Default PEC	Median	2.5 Percentile	97.5 Percentile	**Assessment Factor**	Median	2.5 Percentile	97.5 Percentile	**Assessment factor**
Free in Air	3E-11	7E-12	2E-14	4E-10	**2E+04**	2E-11	1E-13	2E-10	**1E+03**
Bioavailable in air	4E-11	7E-11	1E-12	1E-09	**1E+03**	2E-10	6E-11	5E-10	**8E+00**
Total in Air	4E-11	7E-11	1E-12	1E-09	**1E+03**	2E-10	6E-11	5E-10	**8E+00**
Free In Water	2E-9 3E-6	8E-09	3E-11	3E-06	**9E+04**	4E-08	3E-09	3E-07	**8E+01**
Bioavailable in Water	3E-6	1E-06	7E-09	5E-04	**6E+04**	7E-06	8E-07	2E-05	**3E+01**
Total in Water		2E-06	8E-09	5E-04	**6E+04**	7E-06	1E-06	2E-05	**2E+01**
Free in Sediment	1E-16	5E-17	2E-21	7E-14	**3E+07**	3E-16	3E-20	1E-14	**4E+05**
Bioavailable In Sediment	5E-10	8E-12	2E-14	6E-09	**3E+05**	4E-11	2E-12	9E-10	**6E+02**
Total in Sediment	3E-9	8E-10	5E-13	2E-06	**4E+06**	3E-09	3E-11	5E-07	**2E+04**
Free In soil	3E-14	2E-14	3E-17	1E-11	**5E+05**	7E-14	2E-15	2E-12	**1E+03**
Bioavailable in soil	2E-11	1E-10	6E-13	5E-08	**8E+04**	6E-10	8E-11	5E-09	**6E+01**
Total In soil	2E-8	2E-09	7E-12	6E-07	**8E+04**	7E-09	1E-09	5E-08	**4E+01**