ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

EMPA
Materials Science & Technology

Dynamic Probabilistic Modelling of Environmental Emissions and Concentrations of Engineered Nanomaterials (ENM)

Tianyin Sun, Nikolaus Bornhöft, Martin Scheringer,
Konrad Hungerbühler, Bernd Nowack

Overview

- Problems and objective
  - Limitations of static model
  - More reliable results of ENM emission and concentration
- Method and data
  - Dynamic probabilistic mass-flow modelling
  - Development of ENM production
  - Lifetime release kinetics of ENM
- Results
  - Mass-flow charts of ENM
  - Evolution of ENM in stocks and annual release
  - ENM concentrations results
- Conclusions

Problems and objective

Problems:

- Unrealistic assumptions and simplifications by static mass-flow model
  - Only one year ENM input into the system
  - Complete ENM release from products for the year when they are produced

Objective:

- Provide more reliable environmental emissions and concentrations of nano-TiO_2, nano-ZnO, nano-Ag and CNT by probabilistic dynamic mass-flow modelling

Method and data for dynamic modelling

Method:

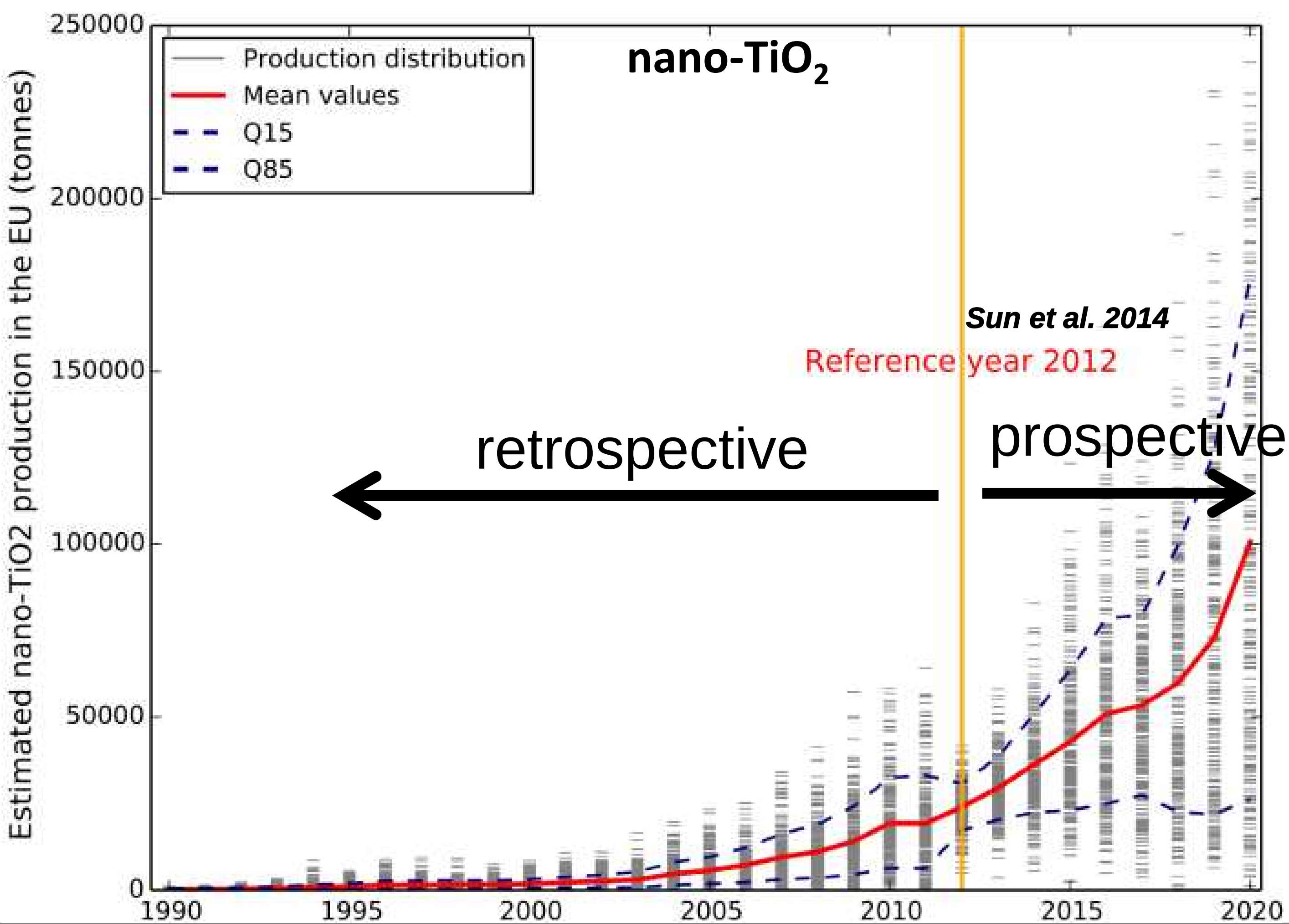
- Adapting the probabilistic dynamic mass-flow model platform developed by Bornhöft et al. 2015 into a model according to need

Data:

- Production: extrapolation and prediction of production development of the four ENM over a period(1990-2020)
- Release kinetics: ENM release from products over time

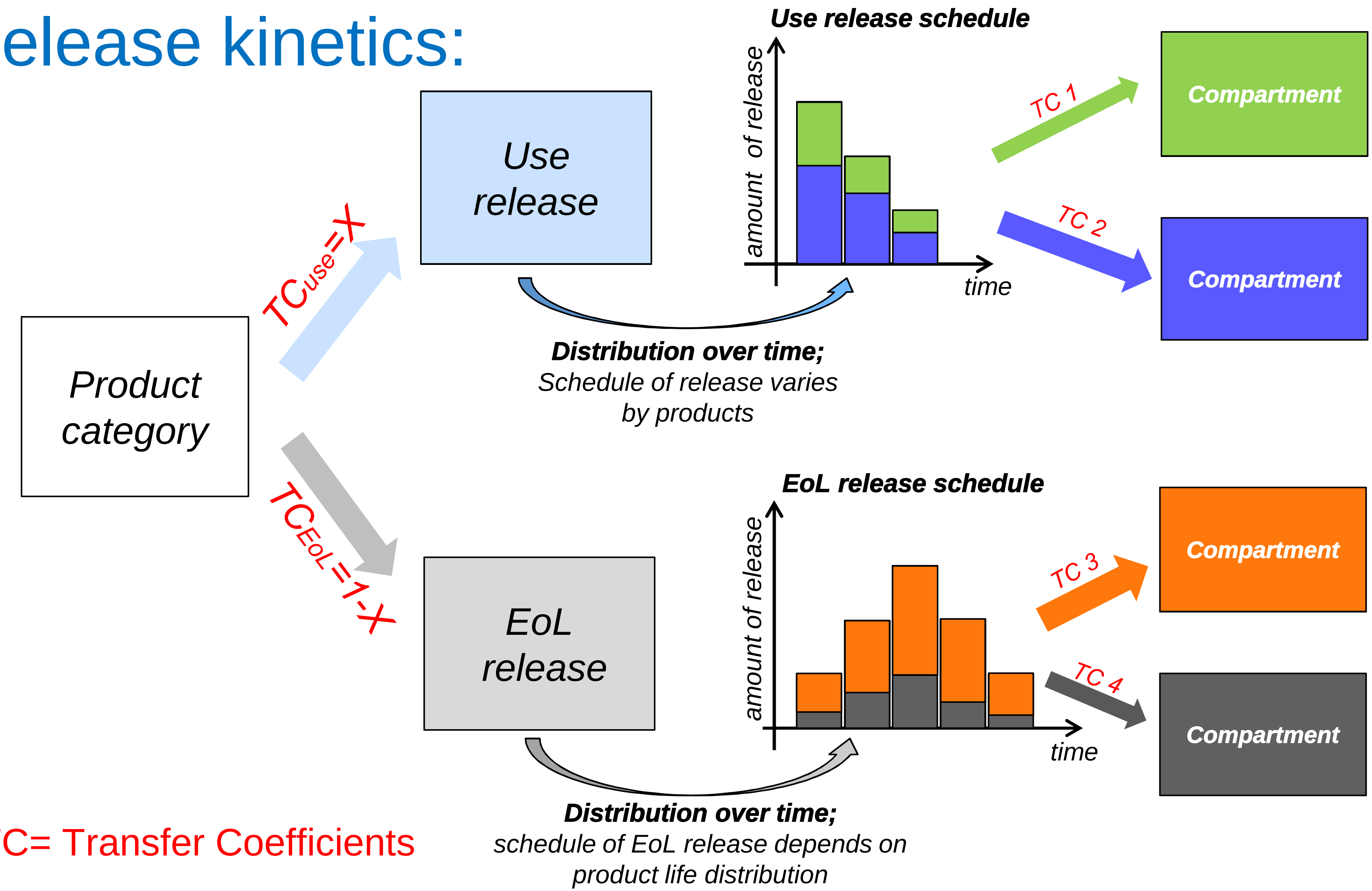
Method and data for dynamic modelling

Production development:



Method and data for dynamic modelling

Release kinetics:

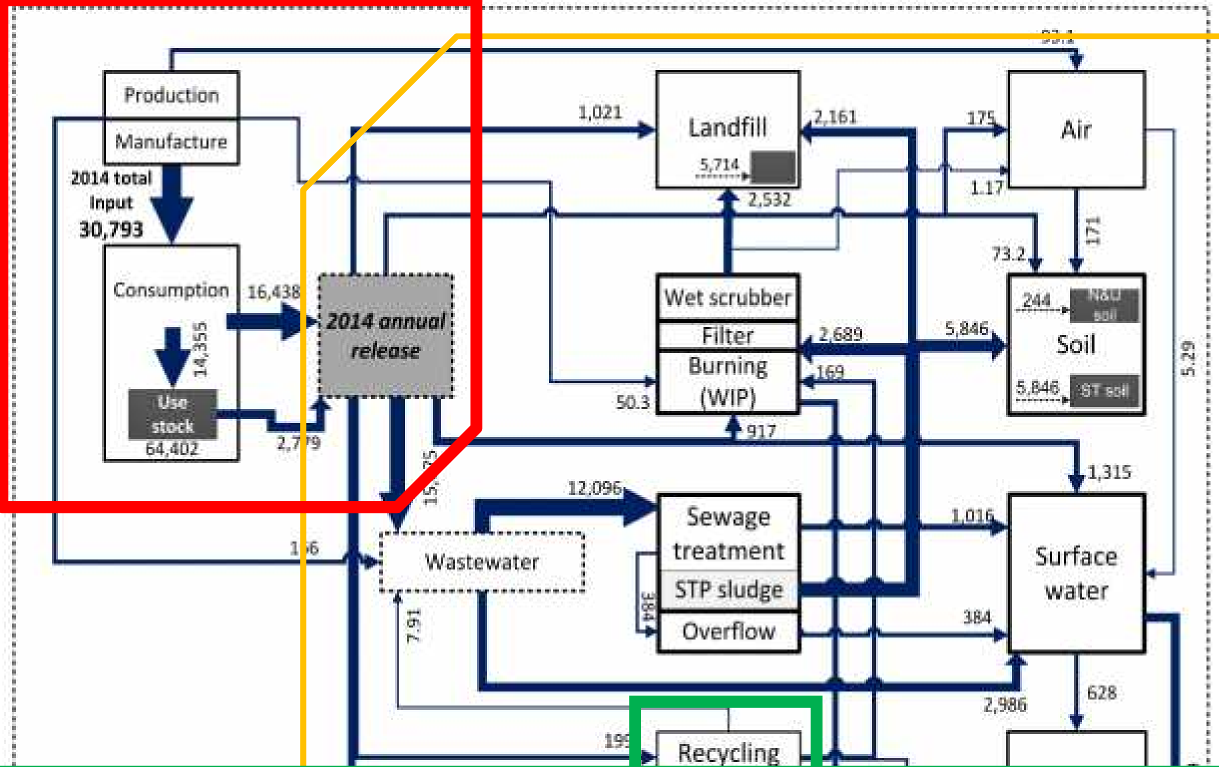


TC= Transfer Coefficients

Results: mass-flow of ENM in the EU

Nano-TiO_2 (2014)

Dynamic components:
1. ***Accumulation in use stock***
2. ***Total annual release***
3. ***Allocations of total annual release***



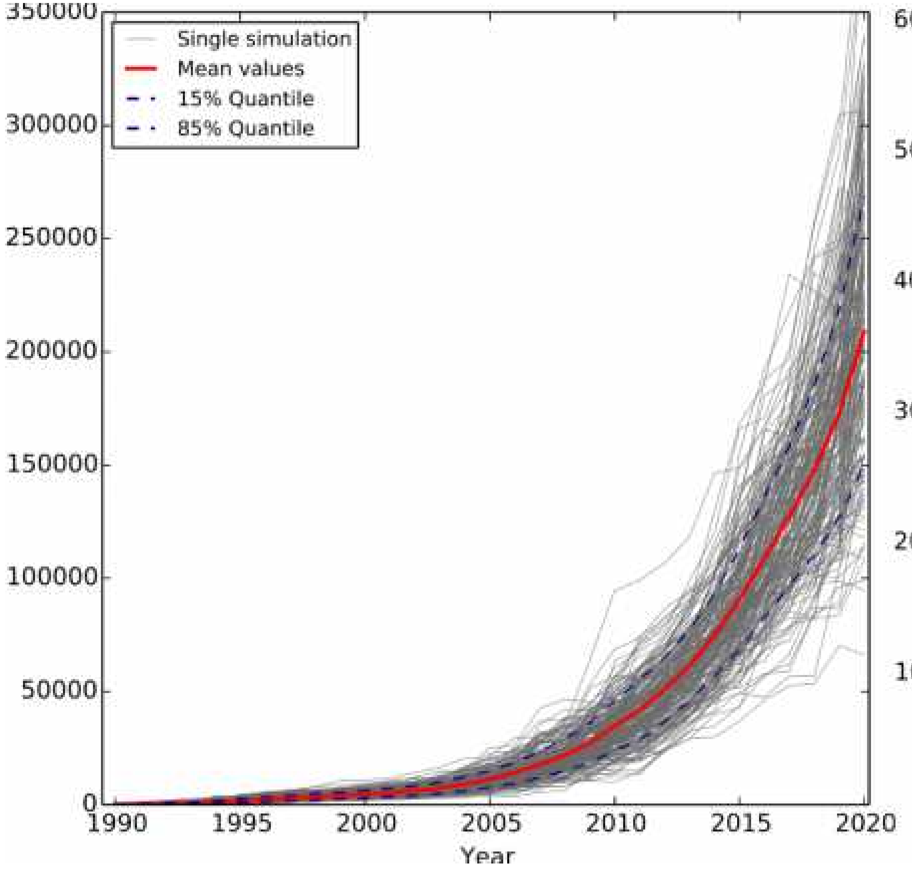
Most transfers from static model Sun et al.2014 are still valid

For ENM fate during recycling process:
Presentation: Session 4A, 15:10-15:40

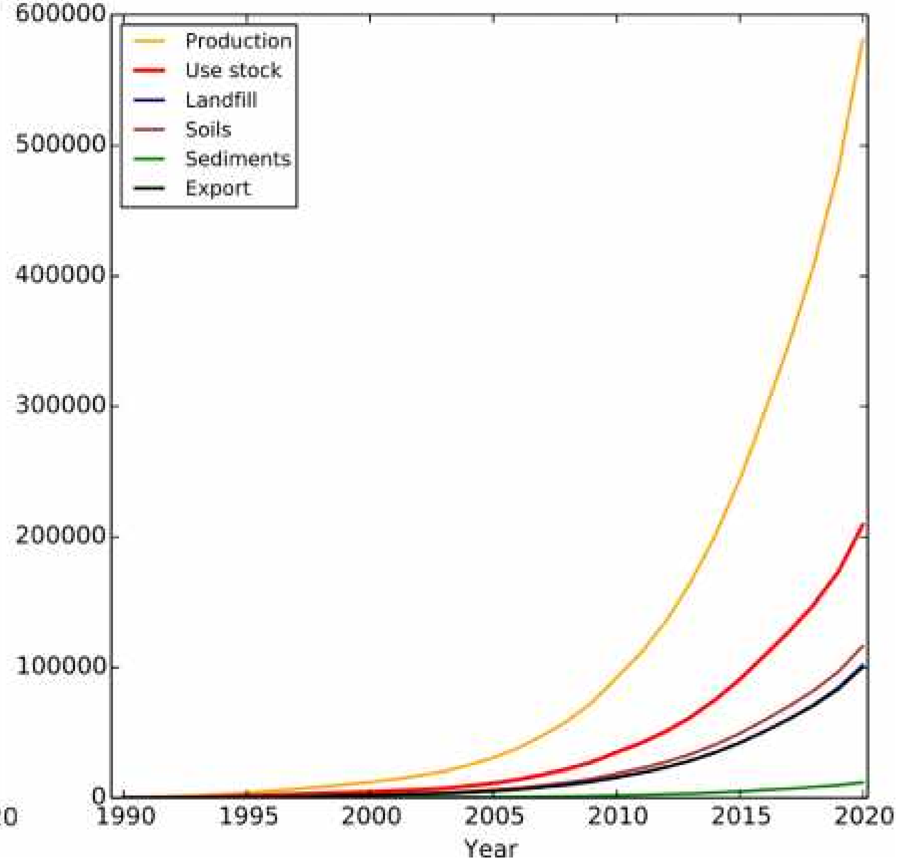
(unit: tonnes)

Results: ENM evolution in stocks

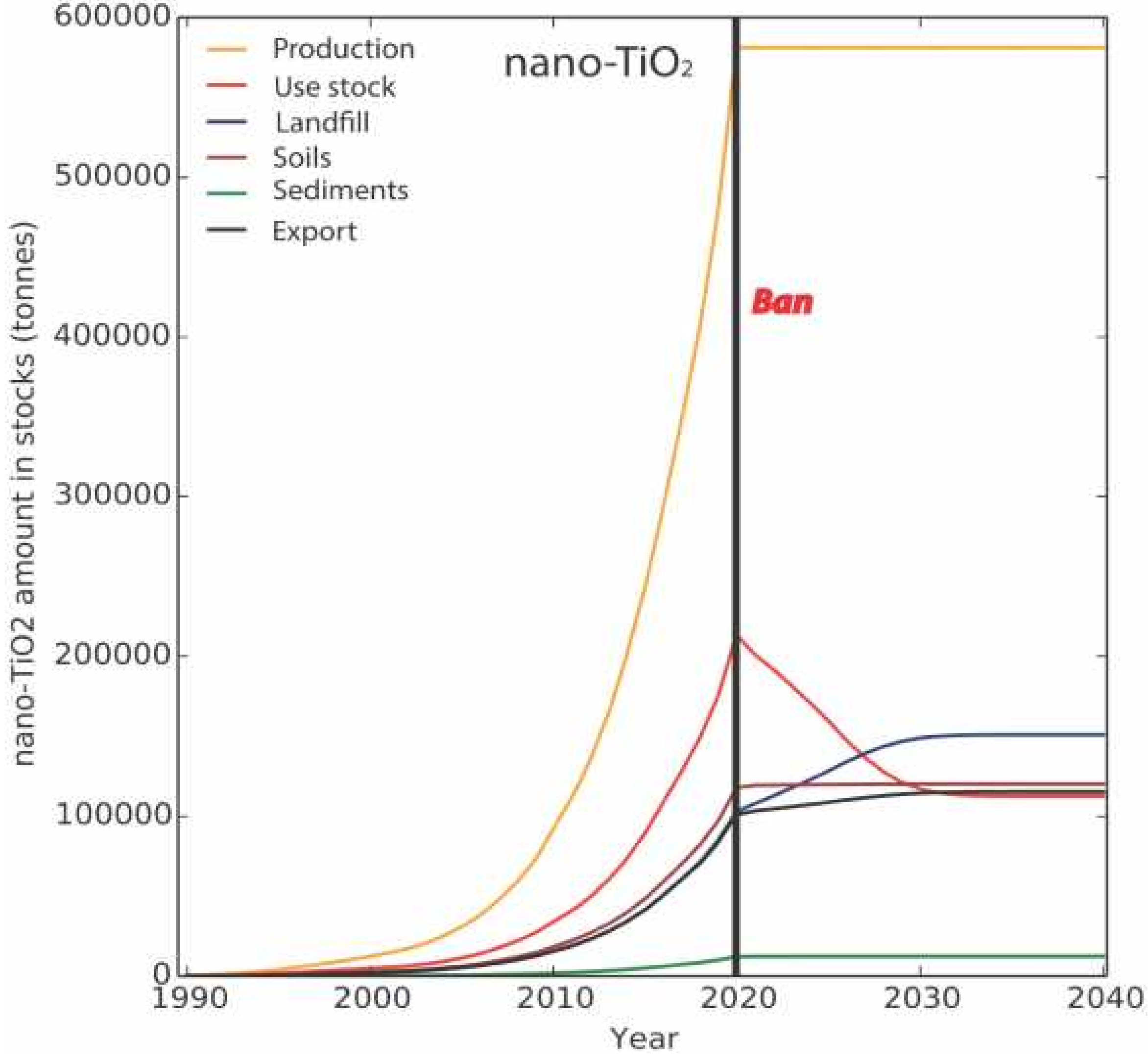
a. nano-TiO_2 in in-use stocks



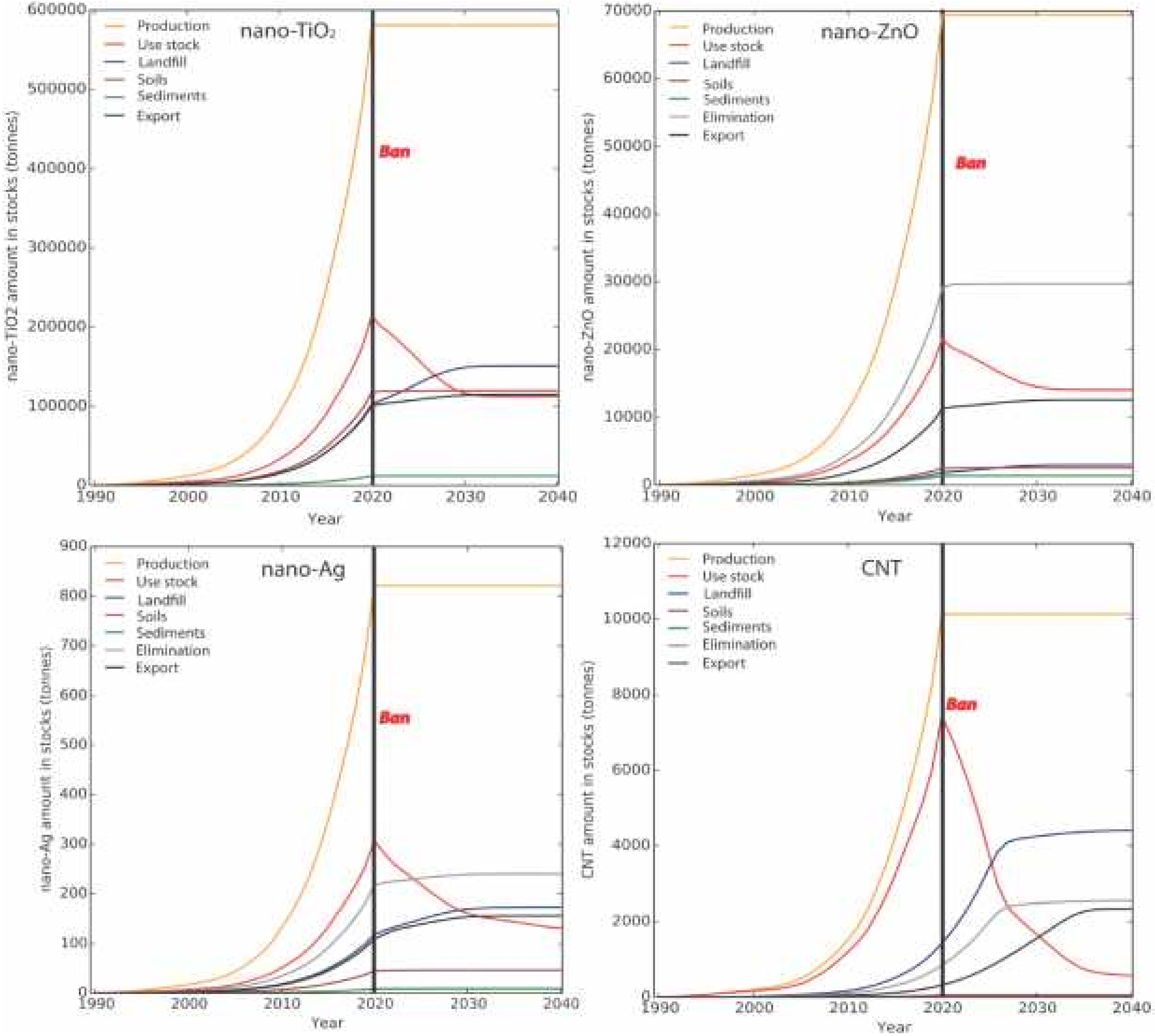
b. nano-TiO_2 in accumulative stocks



Results: Accumulation of ENM production and stocks with hypothesis*(ENM Ban in 2020)*

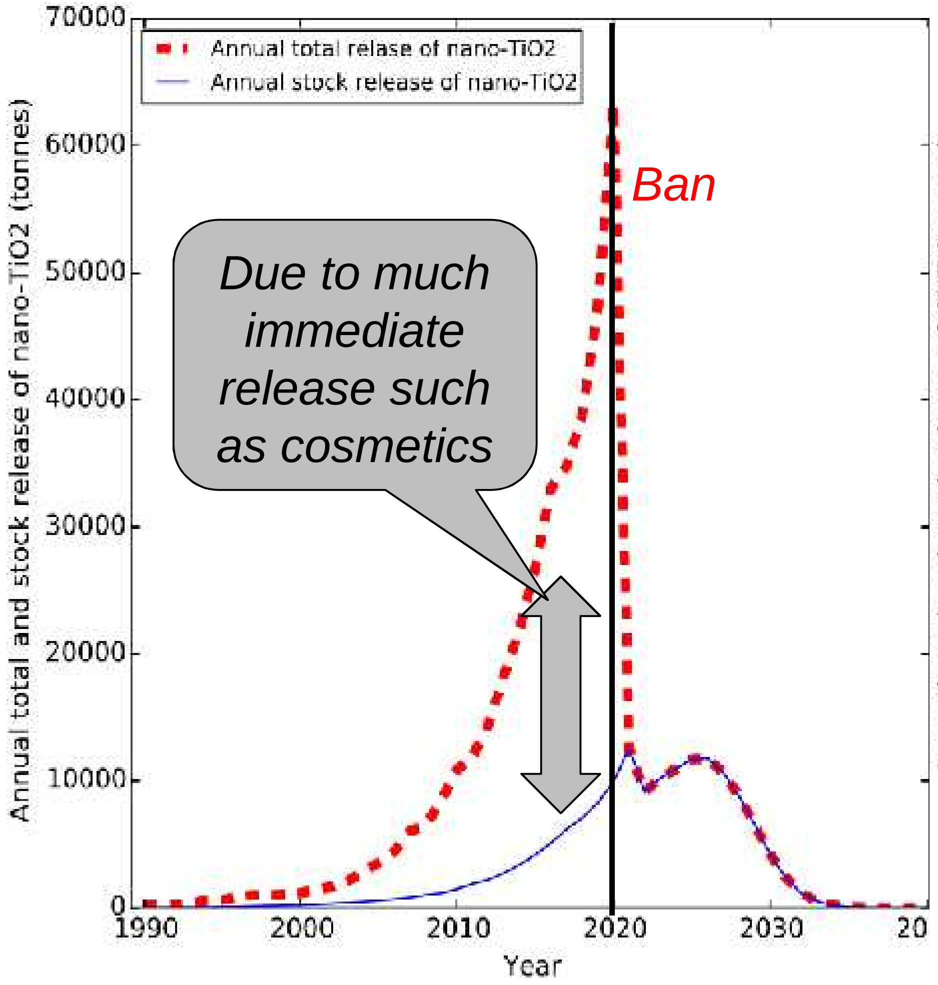


Results: Accumulation of ENM production and stocks with hypothesis*(ENM Ban in 2020)*

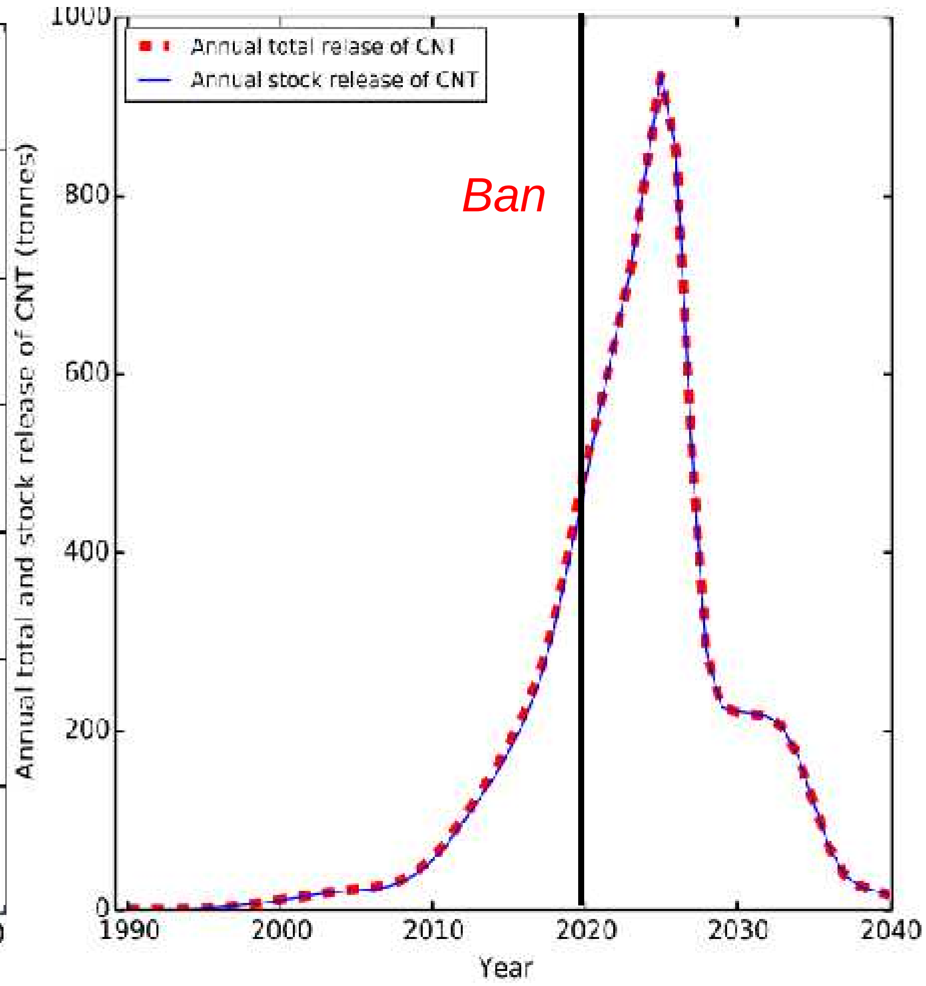


Results: total and stock release with hypothesis *(ENM Ban in 2020)*

a. nano-TiO_2 annual release



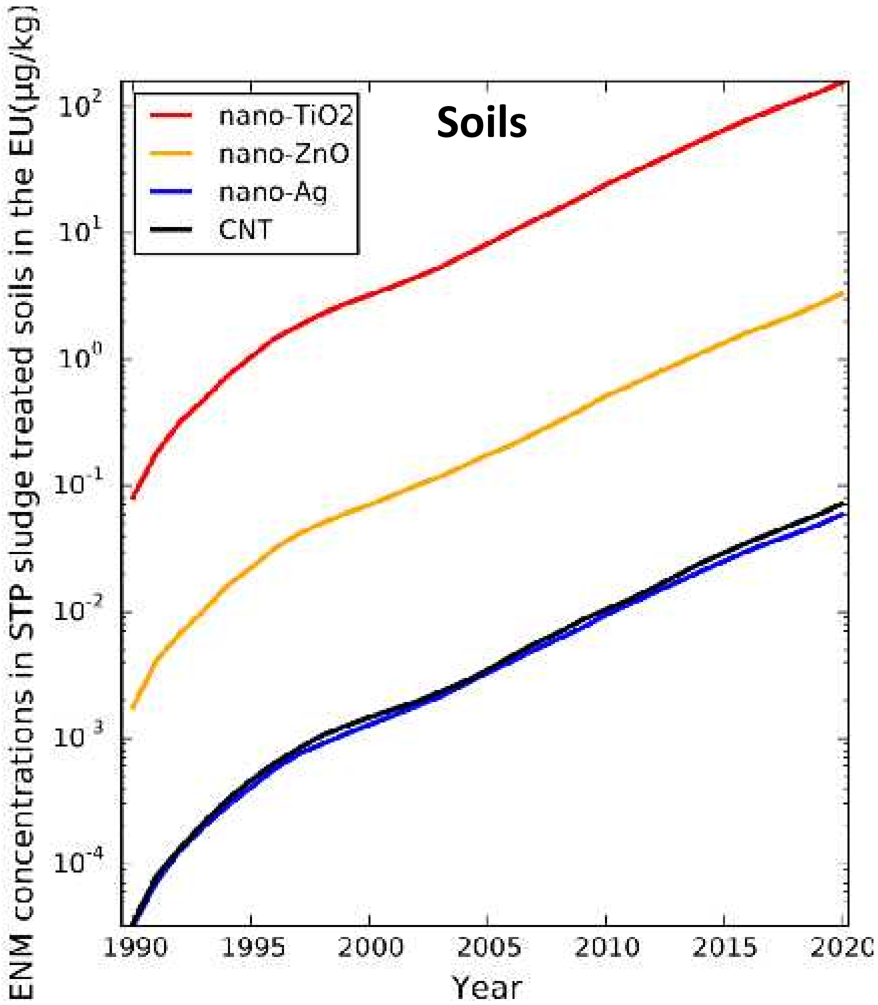
b. CNT annual release

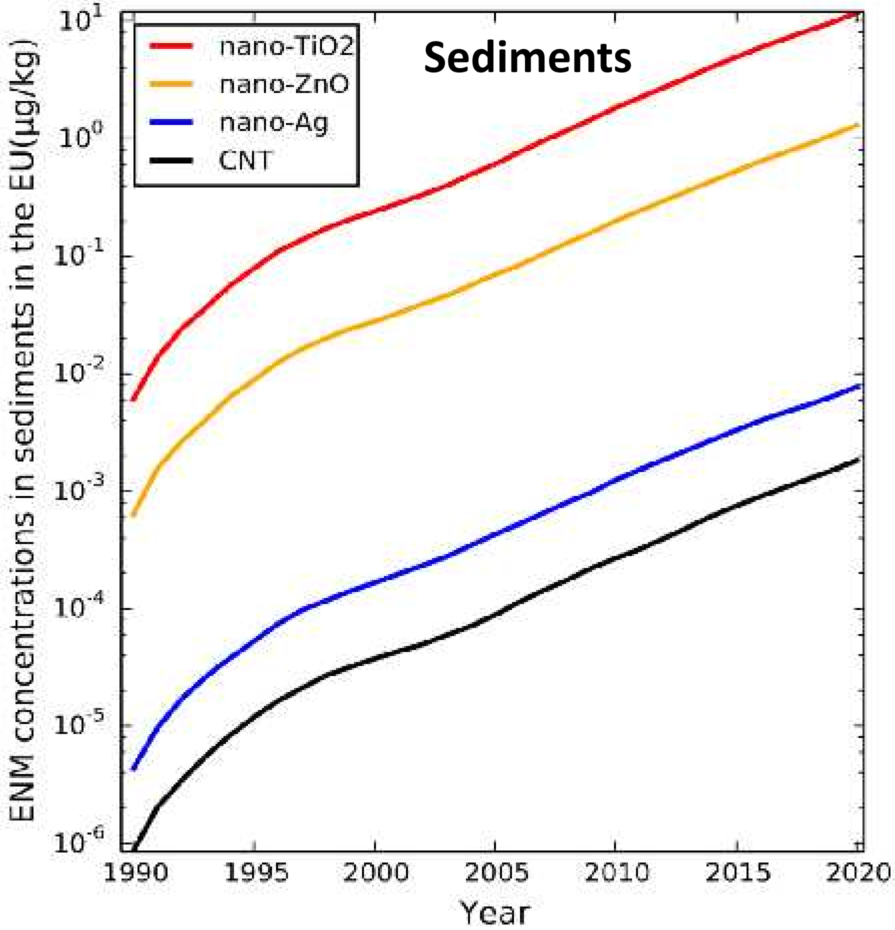


Results: concentrations

Nano-TiO_2	EU (2014) Mean	Mode	Median	$Q_{0.15}$	$Q_{0.85}$	
STP Effluent	**35.1**	**13.9**	26.9	8.60	60.5	µg/L
Surface water	**1.83**	**1.51**	1.68	1.06	2.55	µg/L
Sediment	**3.93**	**4.01**	3.84	2.93	4.92	mg/kg
STP sludge	**1,400**	**1,270**	1,367	820	1,970	mg/kg
Natural and urban soil	**1.93**	**1.44**	1.80	1.26	2.62	µg/kg
Sludge treated soil	**51.5**	**50.3**	51.3	37.8	65.1	mg/kg
Air	**1.22**	**1.30**	1.11	0.70	1.72	ng/m^3
Solid waste	**90.7**	**75.4**	84.8	57.8	125	mg/kg
WIP bottom ash	**444**	**350**	402	263	643	mg/kg
WIP fly ash	**611**	**485**	560	343	881	mg/kg

Results: concentration evolution in soils and sediments





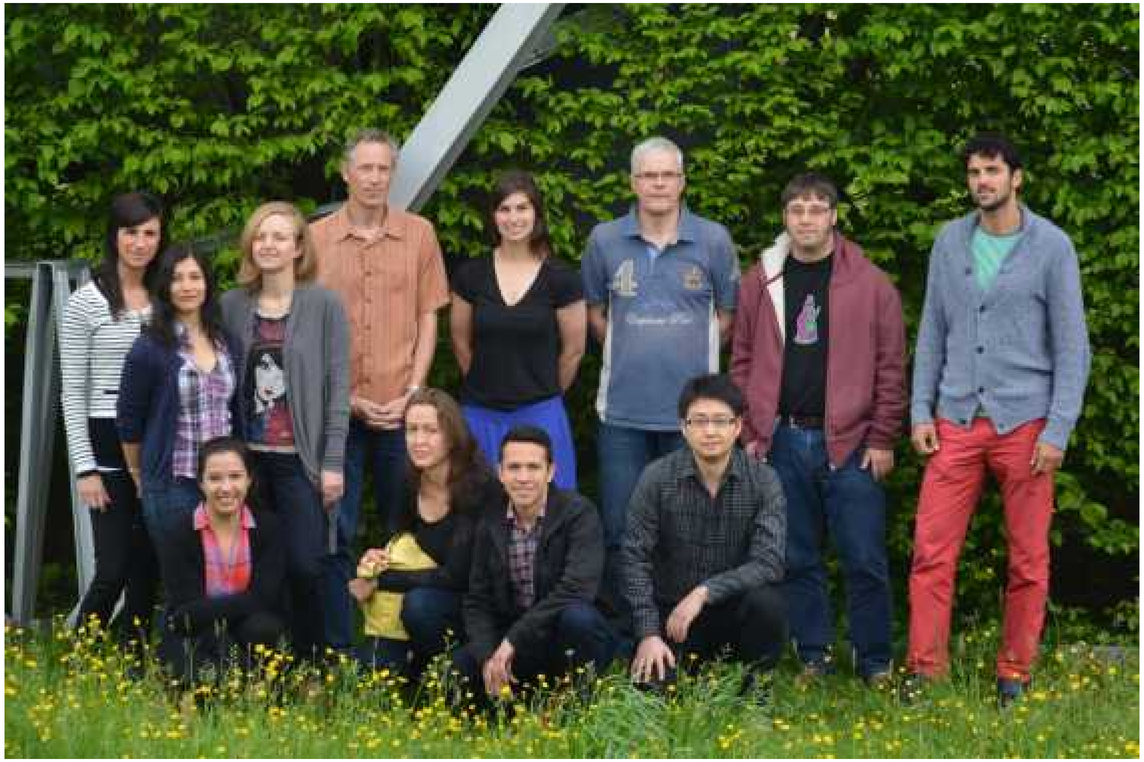
Conclusions:

- With probabilistic dynamic mass-flow model we successfully modeled the emission and concentrations of ENM
- Delay effect varies among ENMs, but all the results show the importance of delay effect, especially for CNT
- Due to some applications e.g. paints in building ENM can be kept in use stock very long
- Latest (and most reliable) ENM concentrations in environmental and technical compartments are given
- For the first time, accumulative (true) ENM concentrations in sinks such as in soils and sediments are given

Acknowledgements:

NRP64

Opportunities and Risks of Nanomaterials
National Research Programme NRP 64



Thank you for your attention!

Contact: tianyin.sun@empa.ch

Data: market projection and patent analysis

lanotechnolgy

Year	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006
Patents analysis																	
Scheu et al. 2006[6]						0.261	0.317	0.328	0.348	0.352	0.452	0.488	0.539	0.724	0.980	1	
Dorsey[7]											0.240	0.301	0.385	0.526	0.769	1	1.137
Parrish 2010[8]												0.457	0.549	0.665	0.814	1	1.243
Daim 2007[9]			0.000	0.000	0.011	0.027	0.016	0.022	0.032	0.033	0.054	0.069	0.106	0.132	0.174	0.248	0.316
Chen 2008 USPO[10]	0.053	0.088	0.077	0.115	0.164	0.166	0.173	0.217	0.277	0.322	0.402	0.497	0.571	0.709	0.788	1	1.260
Chen 2008 EPO[10]	0.063	0.066	0.129	0.096	0.077	0.115	0.184	0.201	0.195	0.255	0.308	0.343	0.387	0.646	0.846	1	1.313
Chen 2008 JPO[10]	0.056	0.042	0.091	0.203	0.322	0.315	0.490	0.455	0.462	0.357	0.378	0.545	0.608	0.587	0.811	1	0.881
Berger 2006[11]												0.254	0.349	0.480	0.673	1	1.398
Dang et al. 2010[12]				0.060	0.087	0.088	0.101	0.108	0.129	0.149	0.190	0.230	0.304	0.445	0.813	1	1.642
Market projection																	

lanotechnolgy

Year	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020
Patents analysis														
Scheu et al. 2006[6]														
Dorsey[7]														
Parrish 2010[8]	1.490	1.727	2.164	2.645	3.341									
Daim 2007[9]	0.410	0.509	0.640	0.770	0.890	1	1.094	1.193	1.246	1.298	1.335	1.366	1.382	1.403
Chen 2008 USPO[10]	1.199	1.564												
Chen 2008 EPO[10]	1.651	1.865												
Chen 2008 JPO[10]														
Berger 2006[11]	1.756	1.851												
Dang et al. 2010[12]	2.183	2.538	2.725	3.253										
Market projection														

Release Kinetics: parameters

Priority (share of the total nano-Ag application)[a]	nano-Ag (product categories)	Use release X	Use release duration (years)	Use release schedule Y1	Y2	Y3	Y4	...	Distribution after use release[b] Waste water	Air	Surface water	Soil	EoL release 1-X	Lifetime distribution (normal) Note: σ is the standard deviation	Distribution after EoL release Landfill	WIP	Recycling	Export
38.1%	Electronics	**0.30**[a]	8[c]	1/8[d]					1.00				**0.70**[a]	mean=8; 3σ=8[c][i][d]	0.09[e]	0.06[e]	0.65[f]	0.2[g]
25.1%	Textiles	**0.60**[a]	3[i]	0.7[h]	0.2[h]	0.1[h]			0.80	0.20			**0.40**[h]	mean=3; 3σ=2[i]	0.31[j]	0.07[j]	0.28[j]	0.34[j]
10.2%	Cosmetics	**0.95**[a]	2[d]	0.9[d]	0.1[d]				0.90		0.10		**0.05**[a]	Y1=0.90, Y2=0.10[d]	0.35[e]	0.25[e]	0.40[k]	
6.6%	Foods	**0.90**[a]	1[d]	1.0[d]					1.00				**0.10**[a]	Y1=1.0[d]	0.6[e]	0.4[e]		
6.0%	Cleaning agent	**0.95**[a]	1[d]	1.0[d]					1.00				**0.05**[a]	Y1=1.0[d]	0.35[e]	0.25[e]	0.40[k]	
3.6%	Medtech	**0.05**[d]	1[d]	1.0[d]					1.00				**0.95**[d]	Y1=1.0[d]		1[d]		
3.3%	Plastics	**0.80**[d]	8[d]	1/8[d]					1.00				**0.20**[d]	mean=8; 3σ=5[d]	0.35[e]	0.25[e]	0.40[k]	
3.0%	Paints	**0.35**[l]	7[m]	0.9[l]	0.1*(1/6)[d][l]				0.50	0.25		0.25	**0.65**[l]	mean=80; 3σ=20[n]	0.3[d]		0.7[o]	
2.4%	Metals	**0.05**[a]	20[d]	1/20[d]					1.00				**0.95**[a]	mean=20; 3σ=5[d]	0.03[e]	0.02[e]	0.95[l]	
0.6%	Glass & Ceramics	**0.35**[l]	10[d]	0.9[l]	0.1*(1/9)[d][l]				1.00				**0.65**[l]	mean=10; 3σ=5[d]	0.20[e]	0.10[e]	0.7[p]	
0.6%	Soil remediation	**0.98**[d]	1[d]	1.0[d]								1.00	**0.02**[d]	Y1=1.0[d]	0.6[e]	0.4[e]		
0.3%	Filter	**0.30**[a]	8[m]	1/8[d]					0.80	0.20			**0.70**[a]	mean=8; 3σ=8[m]	0.09[e]	0.06[e]	0.65[f]	0.2[g]
0.2%	Diapers	**0.05**[d]	1[d]	1.0[d]					1.00				**0.95**[d]	Y1=1.0[d]		1[d]		
0.1%	Paper	**0**[d]											**1.00**[d]	mean=5; 3σ=4[d]	0.07[e]	0.03[e]	0.7[q]	0.2[q]

(a) Sun et al. 2014[12] (b) Revised based on Sun et al.2014[12] (c) SWICO report[31] (d) Expert judgement[32] (e) EEA 2011[33] (f) Kiddee et al. 2013 [34]
(g) EEA 2012[35] (h) Limpiteeprakan et al. 2014[30] (i) Webpage[36] (j) FOE 2013[37] (k) EEA website [38] (l) Kaegi et al. 2010[24]
(m)ATD Home inspection[39] (n) nano-House project[40] (o) EEA 2009[41] (p) Glass International [42] (q) ERPC[43]
Note: Yn = year n, e.g. Y1= year 1