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New developments in assessing environmental flows of nanomaterials

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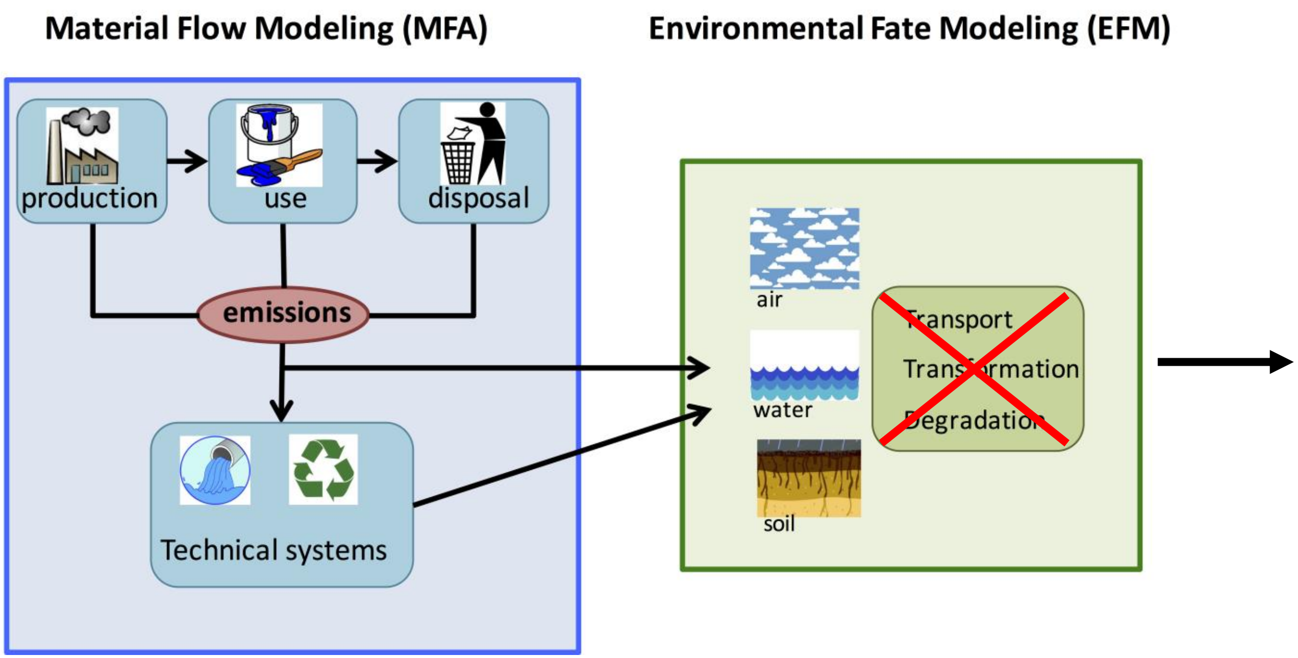
Exposure Assessment

- Material flow models (MFA) predict releases from products, fate in technical systems and final release to the environment
- Environmental fate models (EFM) describe the further fate in the environment and distribution within environmental compartments



Simplified PEC-values, worst-case (no further degradation)

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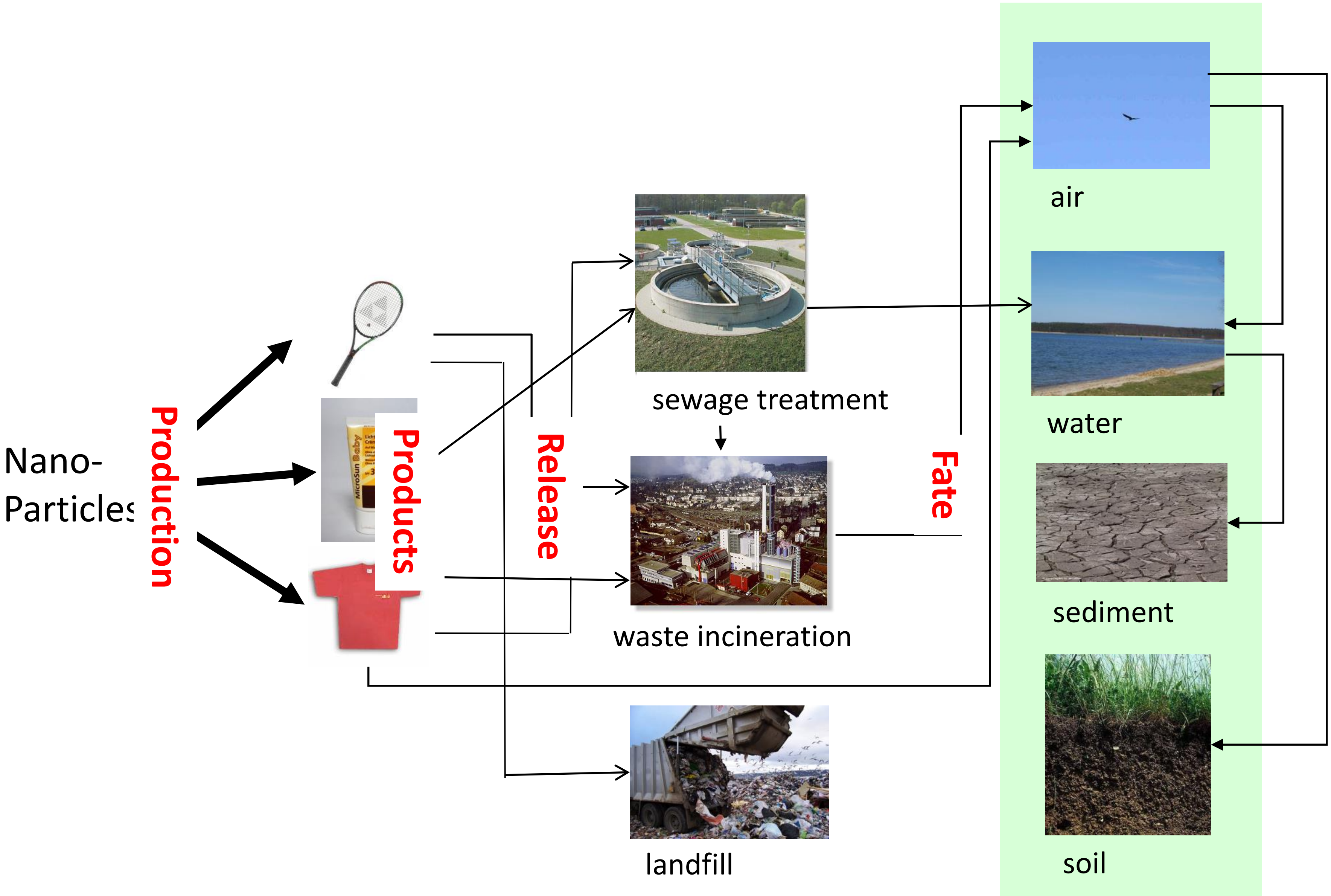
Modeling flows to the environment



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Input data required for MFA

Parameter	Comment	Uncertainty
Production volume within the system boundary	Directly available or scaled up/down from other regions	Depending on the material the uncertainty is medium to very high
Distribution of mass to product categories	The most critical parameter in MFA	Very high: quantitative data are largely absent
Release from products/ applications	Transfer factors needs to be estimated based on release studies or expert knowledge	Real-world studies using real products are mostly missing, therefore quite high uncertainty. Often worst-case assumptions are used.
Transfer factors for technical compartments	Data for WWTP are abundant, for WIP only few available, almost nothing for landfills	Low uncertainty for WWTP and WIP, high for landfills
Transfer factors during recycling	Only considered in some models, no quantitative data available	Uncertainty medium
Transfer factors for environmental compartments	Although transfer between environmental compartments is part of EFM, some MFA models include limited transfers	Often worst-case scenarios

Nowack (2017) *NanoImpact* **8:** 38-47

MFA models

Model name	Reference	Model type	Uncertainty consideration	ENM
PEC estimation	(Boxall et al., 2007)	Simple algorithms	3 scenarios	11 ENM
MFA	(Mueller and Nowack, 2008)	Excel-based MFA	2 scenarios	TiO_2, CNT, Ag
PMFA	(Gottschalk et al., 2010)	Probabilistic model in R	Probabilistic	TiO_2, ZnO, Ag. CNT, fullerenes, SiO_2, Au, Fe-oxides
nanoPoll	(O'Brien and Cummins, 2010a)	Excel with add-on packages	Probabilistic	TiO_2, Ag, CeO_2
PFA	(Arvidsson et al., 2012)	Implemented in Excel	Scenarios	Ag, TiO_2
LEARNano	(Keller et al., 2013; Liu et al., 2015)	Integrated in RedNano, web-based	Scenarios	10 ENM
DPMFA	(Bornhöft et al., 2016)	Dynamic probabilistic model in Python	Probabilistic	TiO_2, CNT, Ag, ZnO
PMFA Version 1.0.0	(SUN, 2016)	Probabilistic model in R with GUI (graphical user interface)	Probabilistic	CuO, DPP, iron oxides

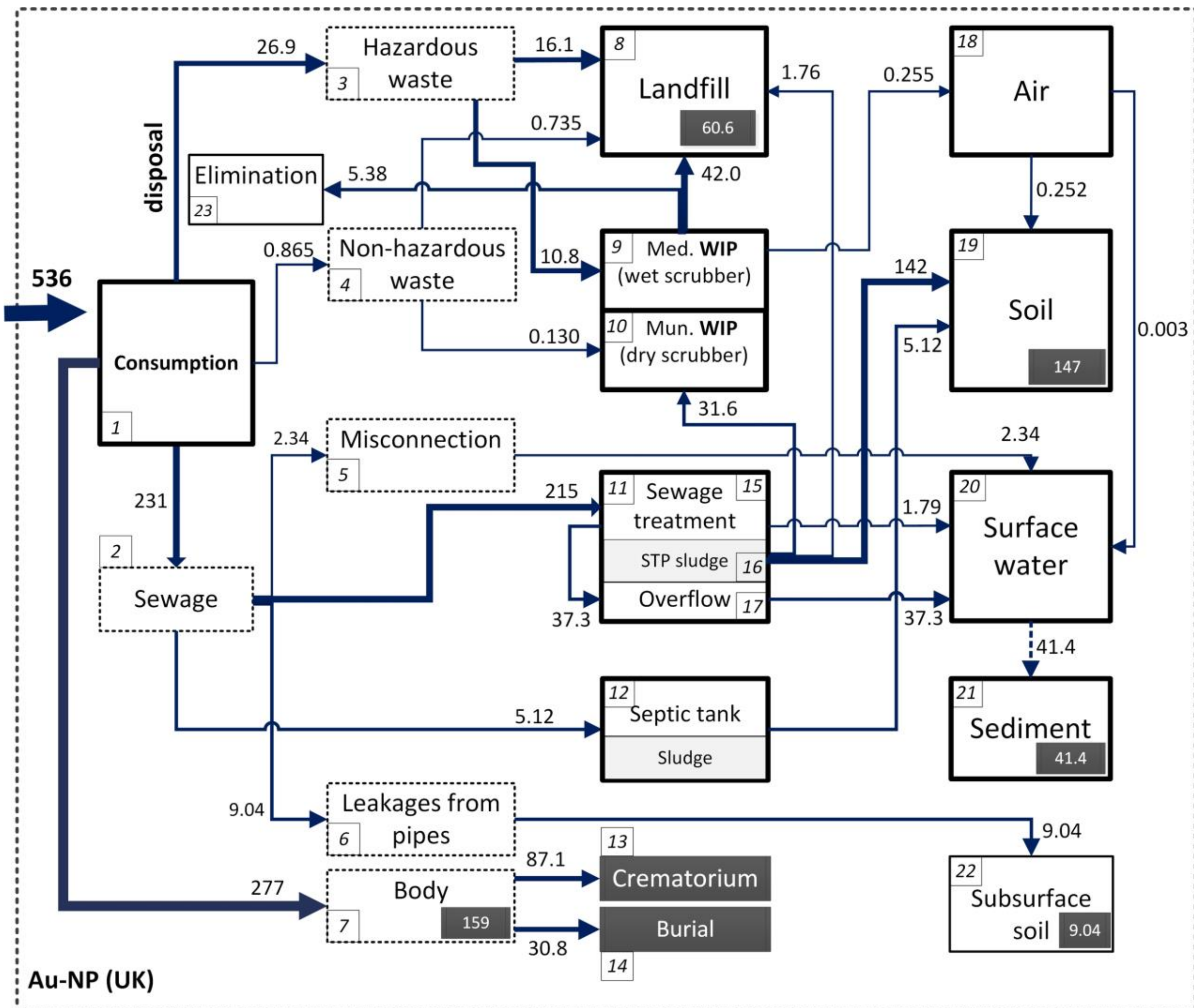
Nowack (2017) *NanoImpact* **8:** 38-47

Nano-gold: Prospective Flows

- Assessment of potential future flows: Prospective realistic worst-case
- Based on registrations, patents, scientific literature
  - Au-NP enabled medical applications which are approved, in clinical trials or show promise of translation from pre-clinical models
- nano-Au uses
  - in vitro medical devices or devices used for detection of specific disease biomarkers
  - treatment or management a particular disease, for example gum infections, cancer and diabetes

Mahapatra et al. (2015) *J. Nanobiotechnol.* 13: 93

Nano-gold: Prospective Flows



Nano-Au used in medical applications

Prospective scenario

Annual flow of nano-Au in the UK in kg/year

Mahapatra et al. (2015) *J. Nanobiotechnol.* 13: 93

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Nano-gold: Prospective Concentrations

Table 2 Predicted Au-NP concentrations in technical and environmental compartments

	UK				US				Units
	Mean	**Mode**	**Q_{15}**	**Q_{85}**	**Mean**	**Mode**	**Q_{15}**	**Q_{85}**	
STP Effluent	440	360	220	670	140	130	71	200	pg/L
Surface water	470	270	210	730	4.7	4.0	2.7	6.8	pg/L
STP sludge	120	130	94	150	150	150	120	170	µg/kg
Sludge treated soil	*300*	*300*	*230*	*370*	*150*	*150*	*120*	*170*	*ng/kg· years*
Sediment	*290*	*170*	*130*	*450*	*5.0*	*4.5*	*3.0*	*8.0*	*ng/kg·years*
Hazardous waste	77	78	23	130	65	69	20	110	µg/kg
Medical WIP									
Fly ash	270	30	36	530	260	32	36	530	µg/kg
Bottom ash	200	25	27	410	200	26	27	400	µg/kg
Municipal WIP									
Fly ash	72	70	53	92	39	38	31	47	µg/kg
Bottom ash	55	52	39	71	30	27	22	37	µg/kg

Mahapatra et al. (2015) *J. Nanobiotechnol.* 13: 93

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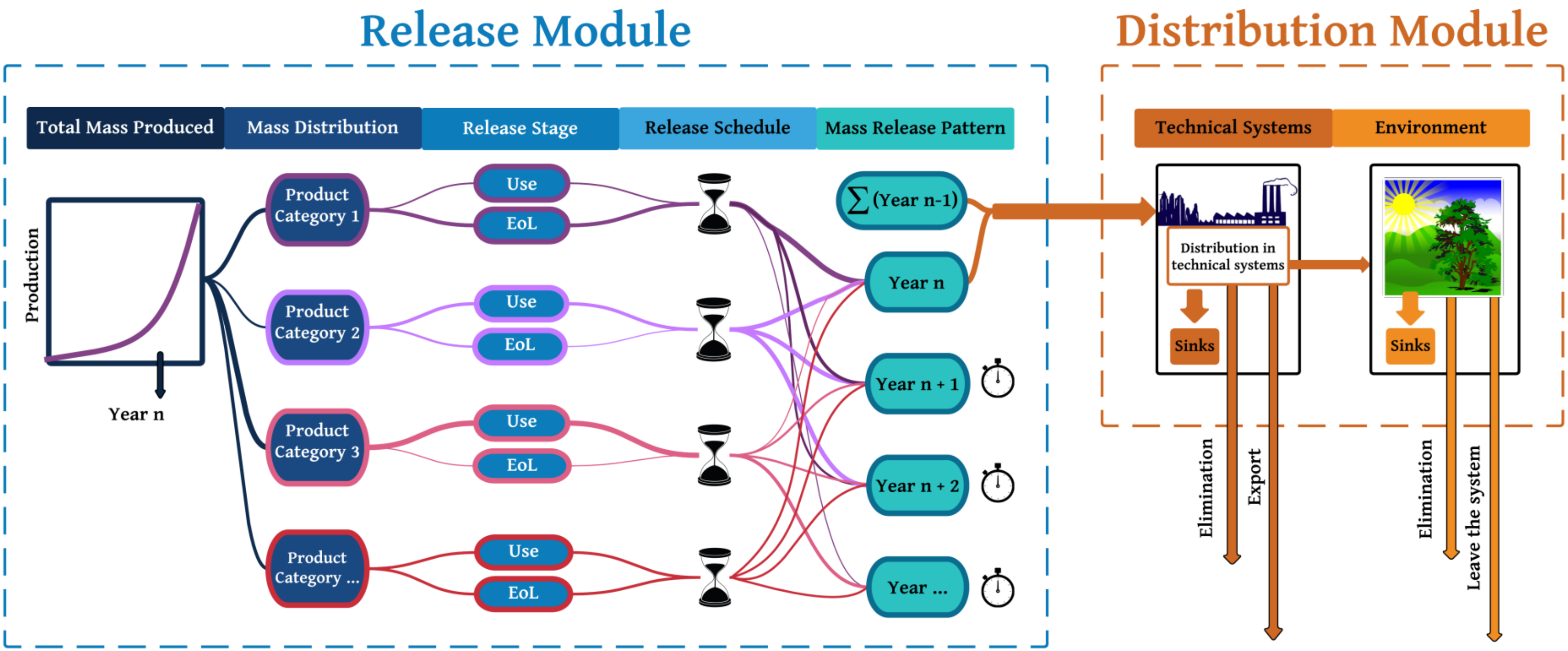
Dynamic vs. static models

- Static models
  - All releases in the same year than produced
  - Equilibrium conditions
- Dynamic models
  - Stocks and sinks included
  - Release kinetics included
  - Life time of products included
  - Tracks the flows over time

Dynamic modeling



Sun et al. (2017) *Environ. Sci. Technol.* **51:** 2854-2863

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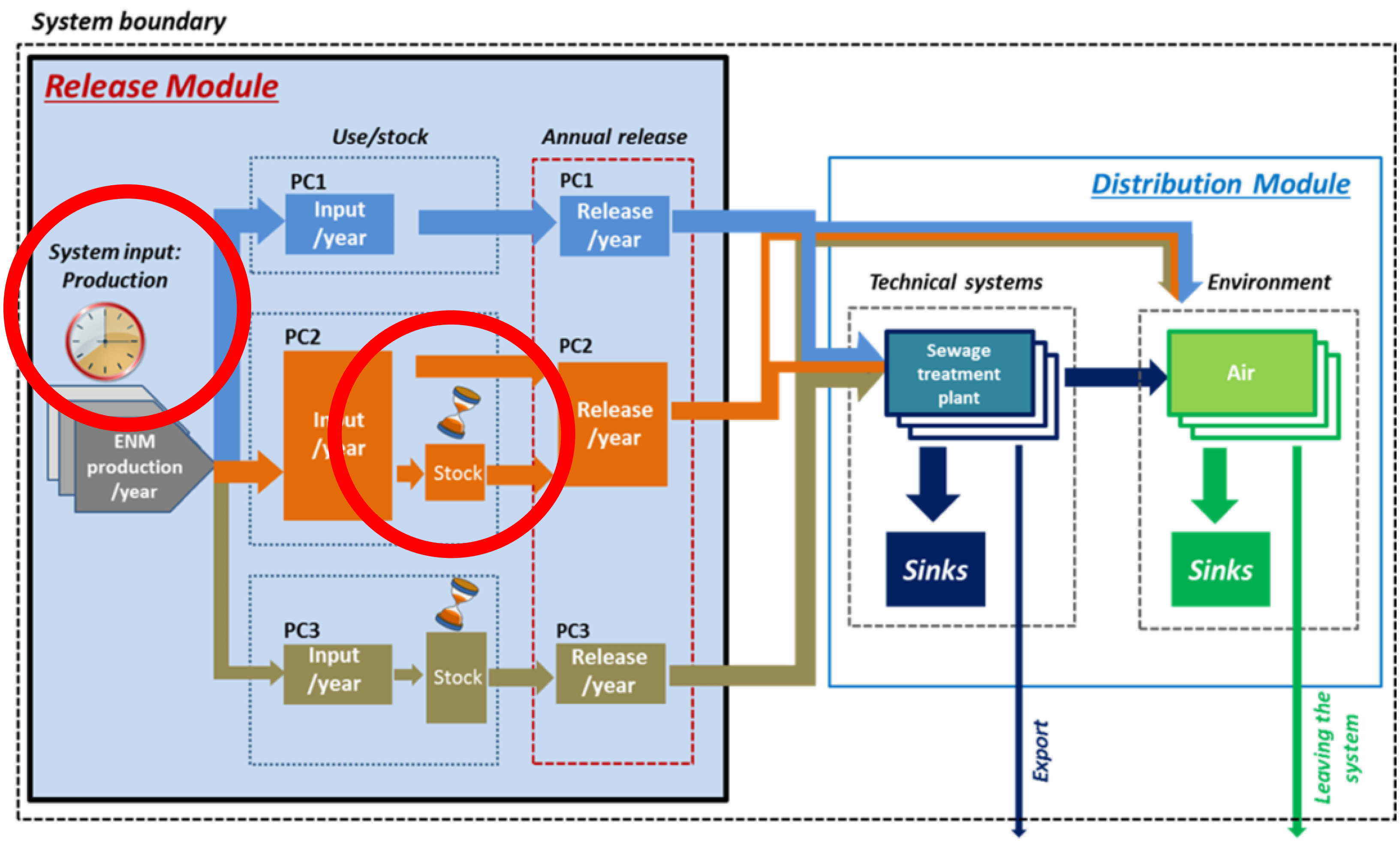
Dynamic MFA



Bornhöft et al. (2016) Environ. Modeling Software 76: 69-80
Sun et al. (2016) *Environ. Sci. Technol.* **50:** 4701-4711

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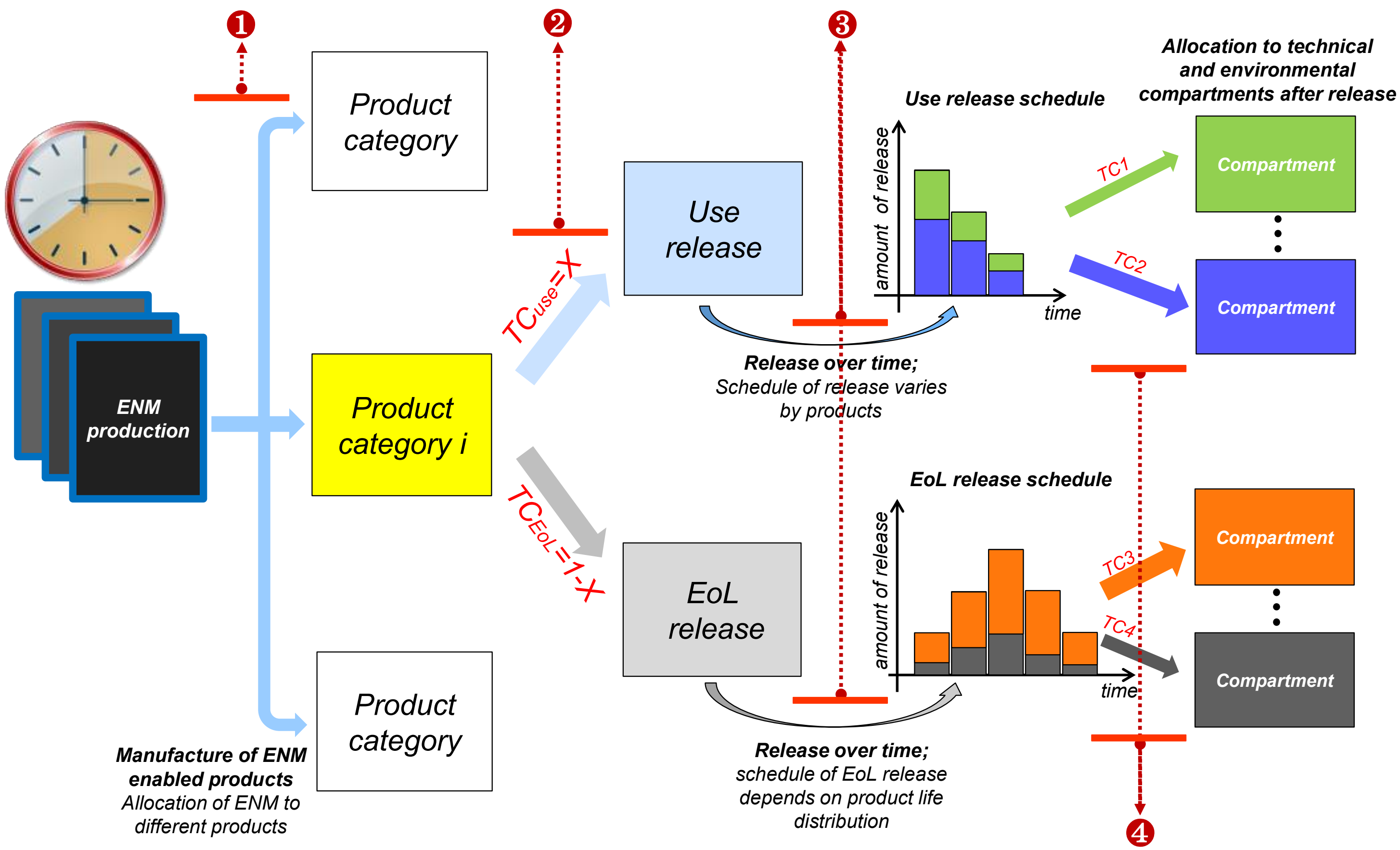
Use release and EoL release



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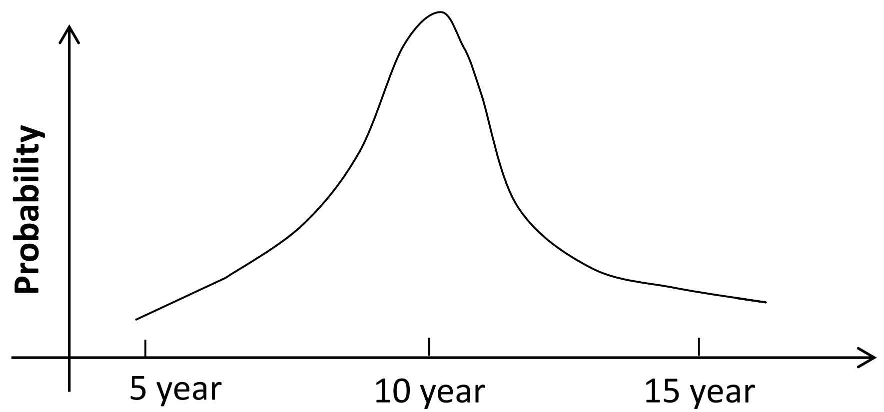
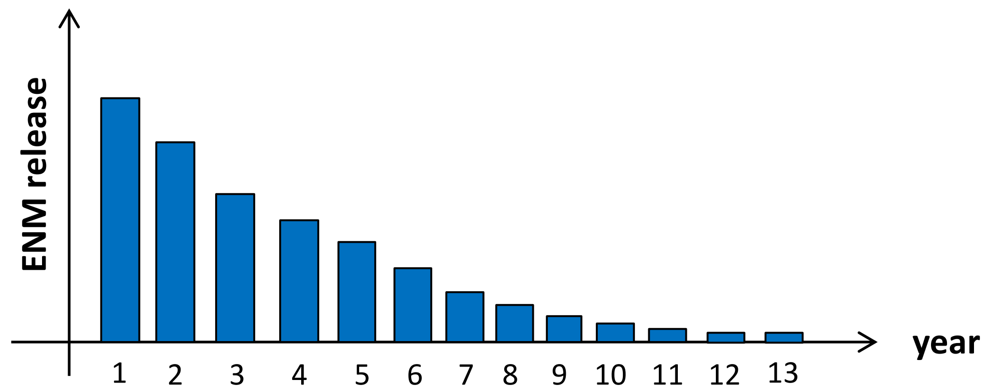
Life time and release kinetics

Release Module: Time dependent ENM release from products

Life span of product category



ENM release kinetic of each product category



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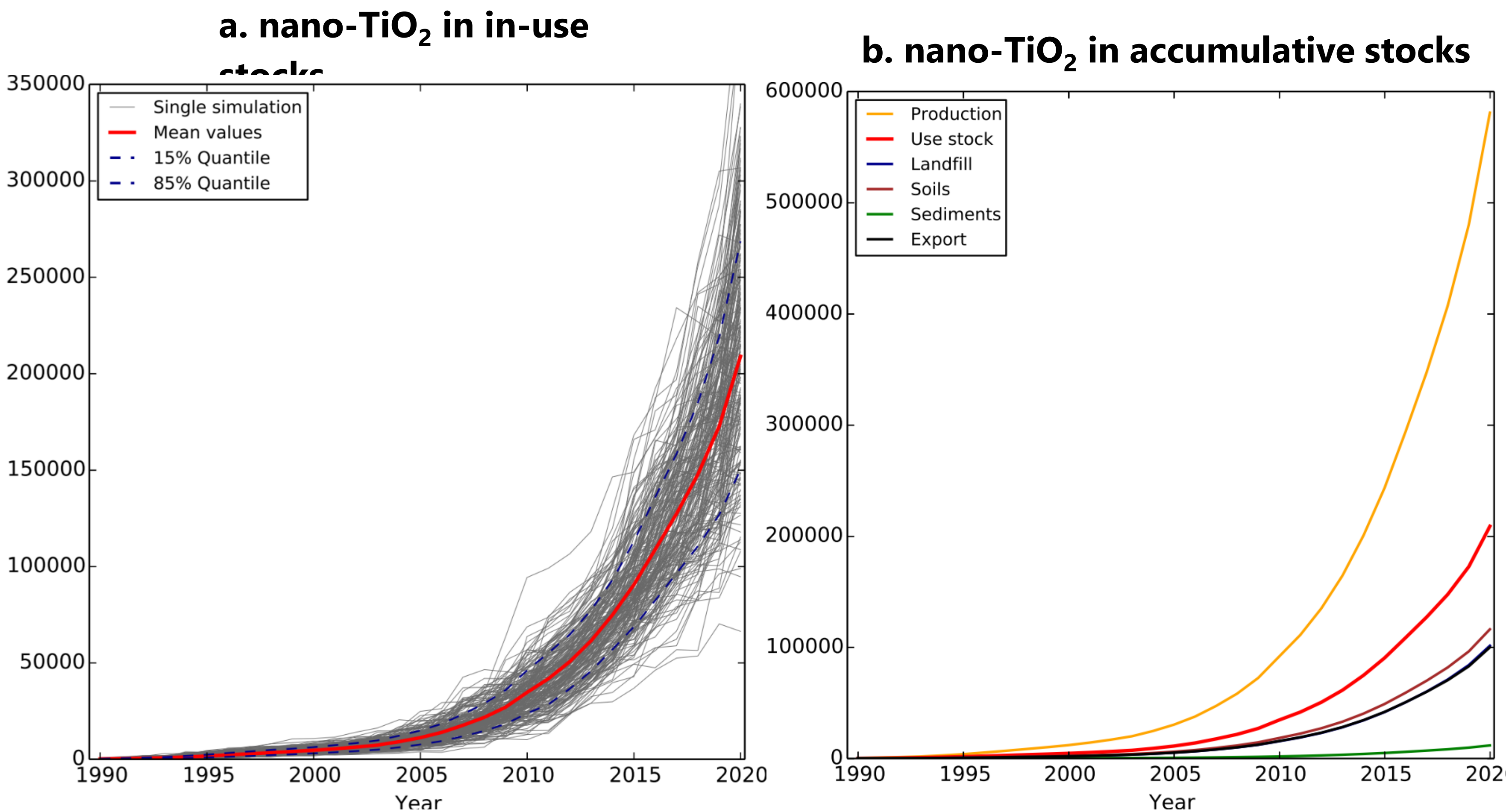
Release Module: Development of ENM in stocks



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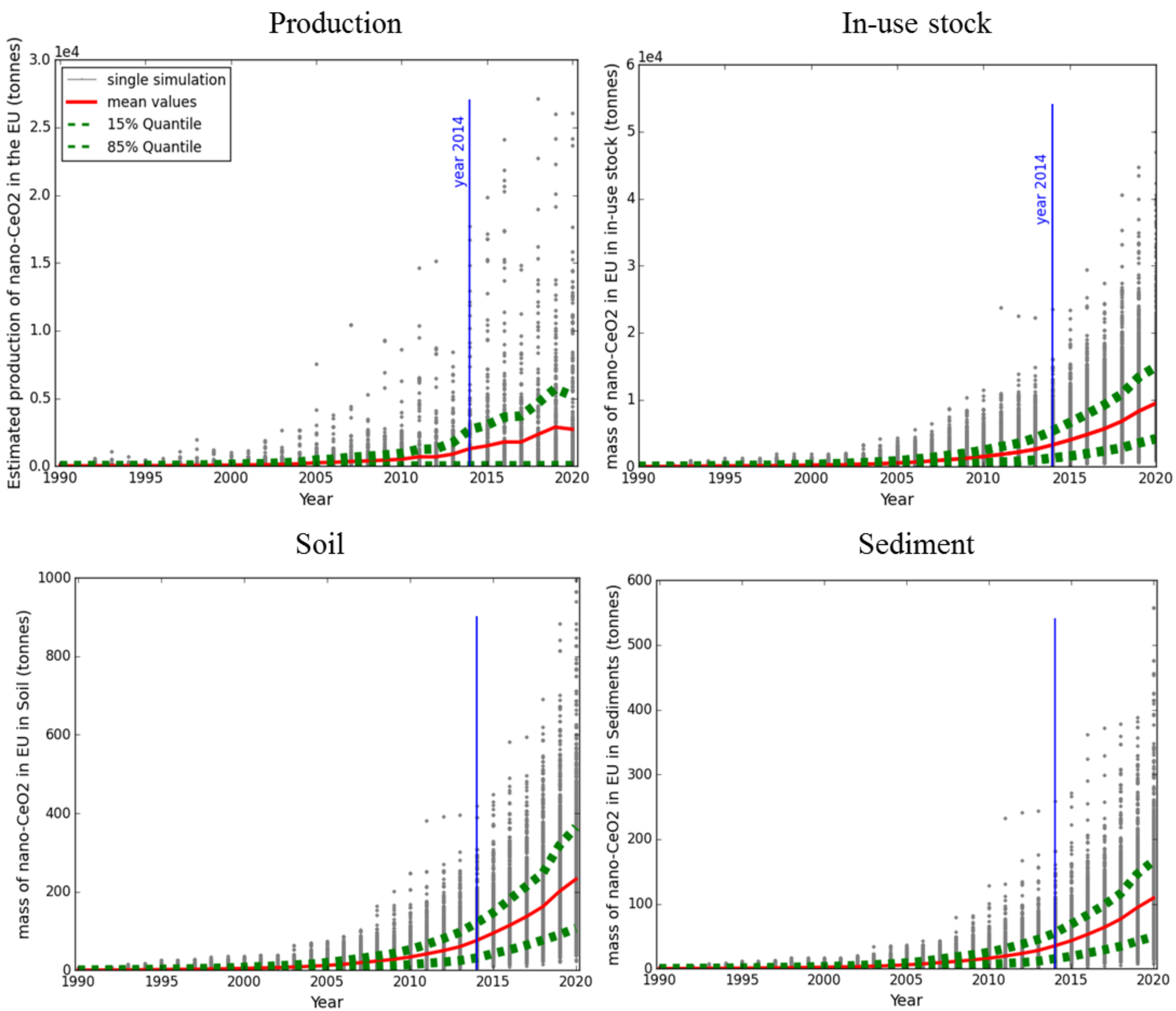
Development of ENM in stocks: CeO_2



Wang et al. (2017) *Environ. Pollut* under revision

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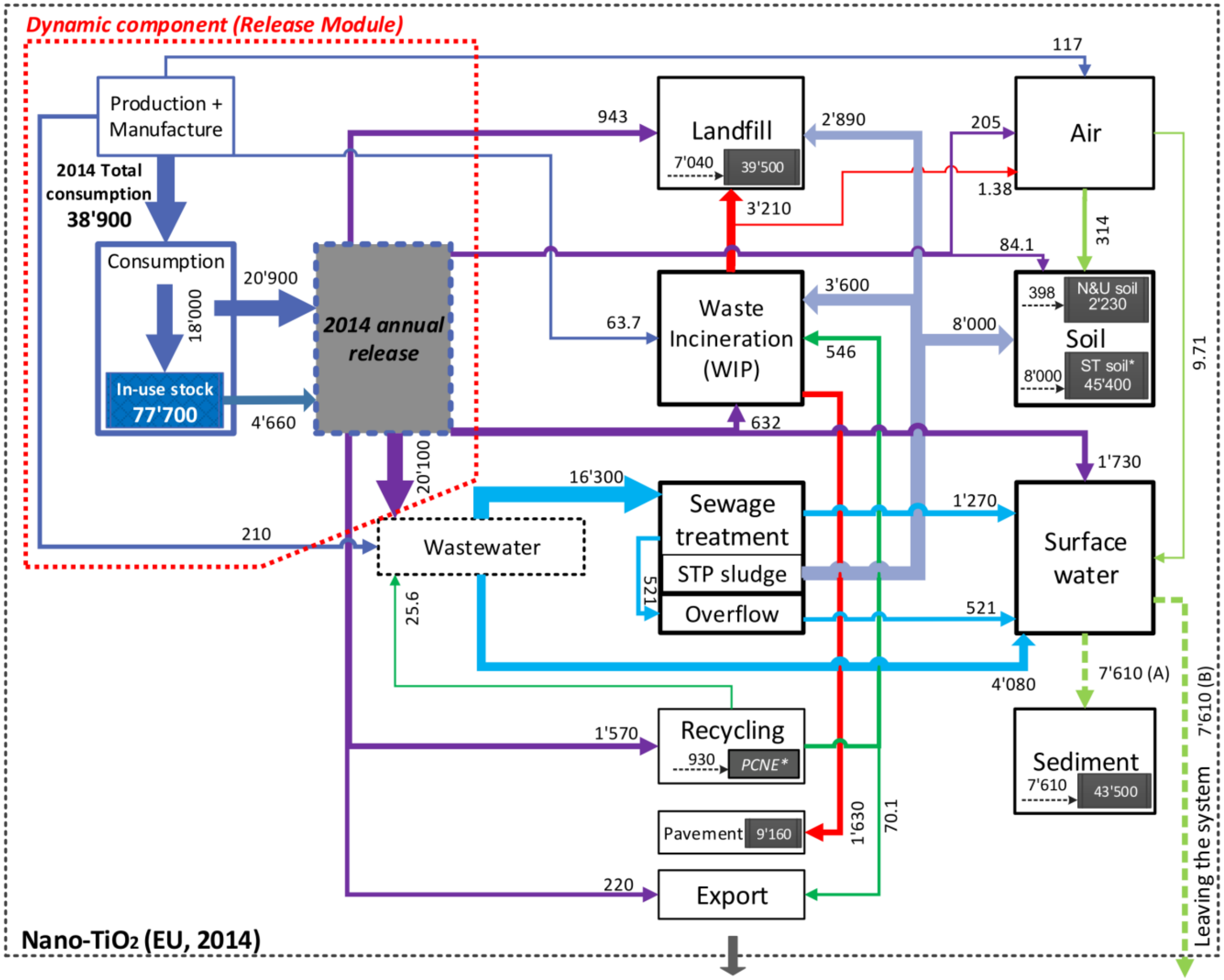
Dynamic TiO_2 modeling



Sun et al. (2016) *Environ. Sci. Technol.* **50:** 4701-4711

Concentrations

	EU (2014)					
	Mean	**Mode**	Median	$Q_{0.15}$	$Q_{0.85}$	
Nano-TiO_2						
STP Effluent	**44.4**	**13.7**	16.3	2.77	76.1	µg/L
STP sludge	**1.60**	**0.47**	0.84	0.16	3.42	g/kg
Solid waste to Landfill	**12.9**	**7.67**	10.3	5.37	21.3	mg/kg
Solid waste to WIP	**10.3**	**6.19**	7.93	4.24	16.9	mg/kg
WIP bottom ash	**395**	**161**	237	93.6	729	mg/kg
WIP fly ash	**543**	**238**	327	129	979	mg/kg
Surface water	**2.17**	**0.61**	1.10	0.19	4.40	µg/L
Sediment	**43.1**	**30.0**	38.7	21.3	65.0	mg/kg
Natural and urban soil	**2.94**	**1.86**	2.57	1.44	4.53	µg/kg
Sludge treated soil	**61.1**	**40.8**	54.6	30.9	93.3	mg/kg
Air	**2.05**	**0.86**	1.24	0.43	3.98	ng/m^3

Sun et al. (2016) *Environ. Sci. Technol.* **50:** 4701-4711

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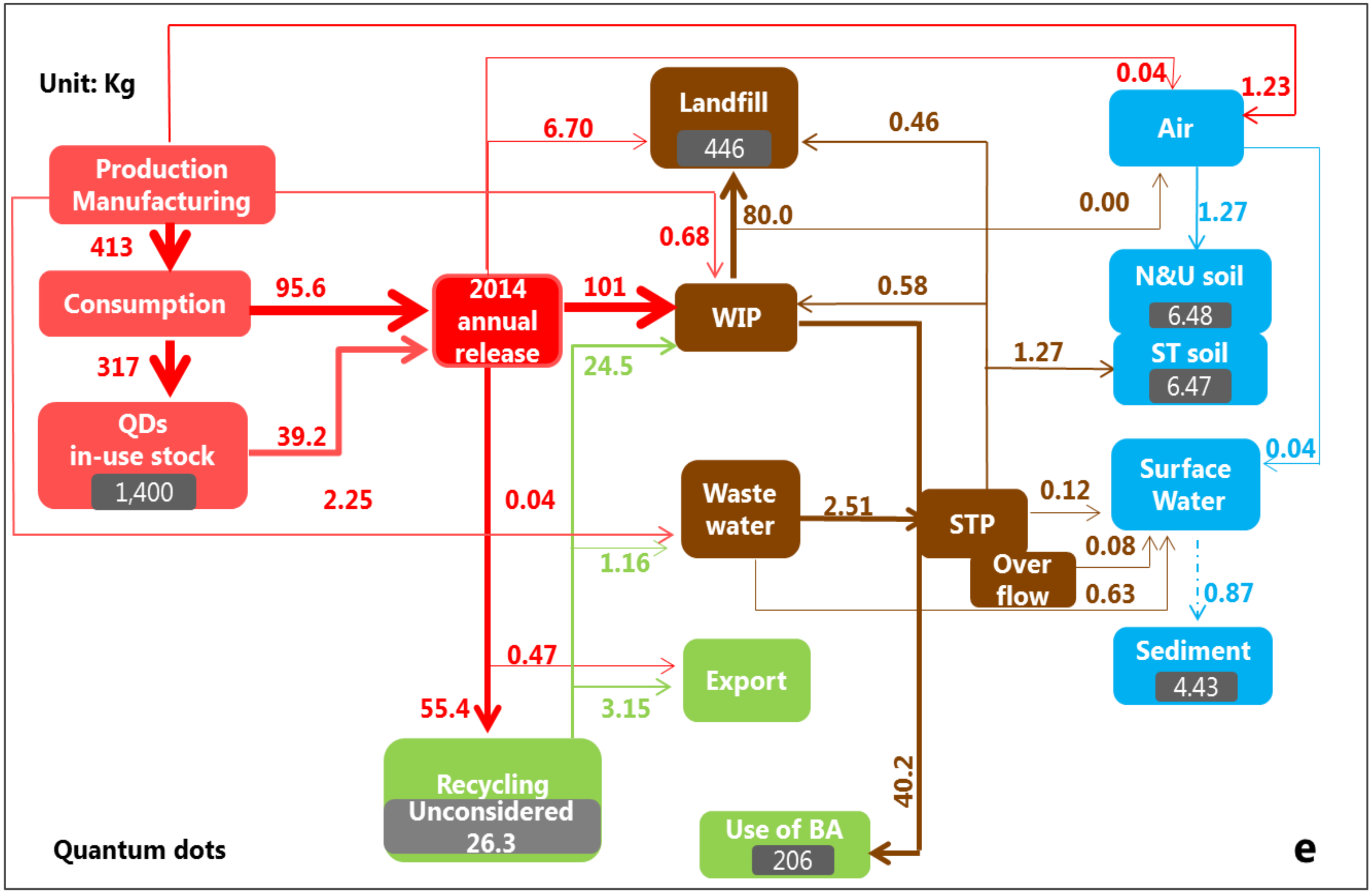
Dynamic QD modeling



Wang et al. (2017) *Environ. Pollut* in revision

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Concentrations

QD concentrations in 2014		
STP Effluent	2.7	pg/L
STP Sludge	0.18	µg/kg
Landfilled waste	91	ng/kg
Incinerated waste	1.6	µg/kg
Bottom ash	8	µg/kg
Fly ash	11	µg/kg
Air	7.9	fg/m3
N&U soil	8.4	pg/kg
ST soil	6.2	ng/kg
Surface water	170	fg/L
Sediment	3.2	ng/kg

Wang et al. (2017) *Environ. Pollut* in revision

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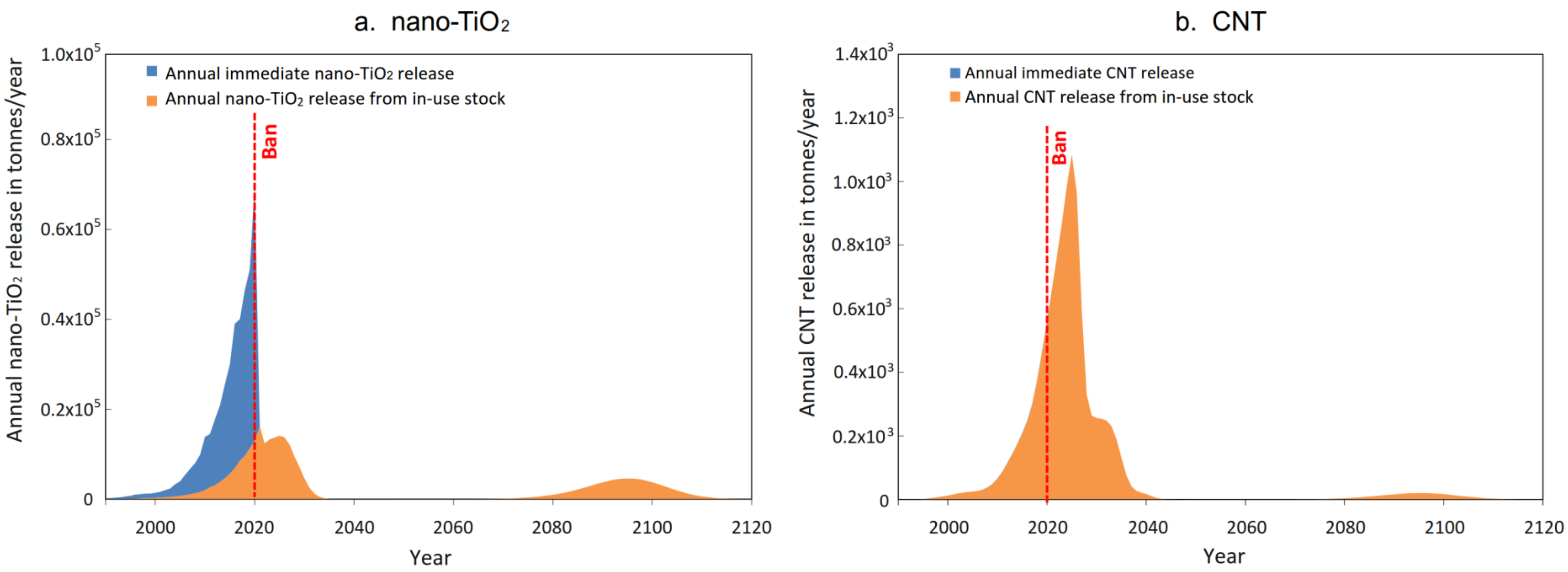
Scenario: Ban of nano in 2020



Sun et al. (2017) *Environ. Sci. Technol.* **51:** 2854-2863

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Different scenarios

Scenarios	Target ENM	Production development and time scope	Application shares of target ENM
Ban of nano-TiO_2 in cosmetics	nano-TiO_2	2015-2020: Production as modelled in Sun et al. (2016), deducting the smaller amount used in cosmetics	The share applied in cosmetics declines from 60% to 0% from 2015 to 2020
Ban of nano-Ag in textiles	nano-Ag	2015-2020: Production as modelled in Sun et al. (2016), deducting the smaller amount used in textiles	The share of application in textiles declines from 25% to 0% from 2015 to 2020
Increase of nano-TiO_2 in concrete	nano-TiO_2	2015-2020: Production as modelled in Sun et al. (2016) adding the increase of application in concrete	The share of application in concrete increase from 0% to 10% from 2015 to 2020
Increase of CNT in tyres	CNT	2015-2020: Production as modelled in Sun et al. (2016) adding the increase of application in tyres	The share of application in tyres increases from 0% to 10% from 2015 to 2020

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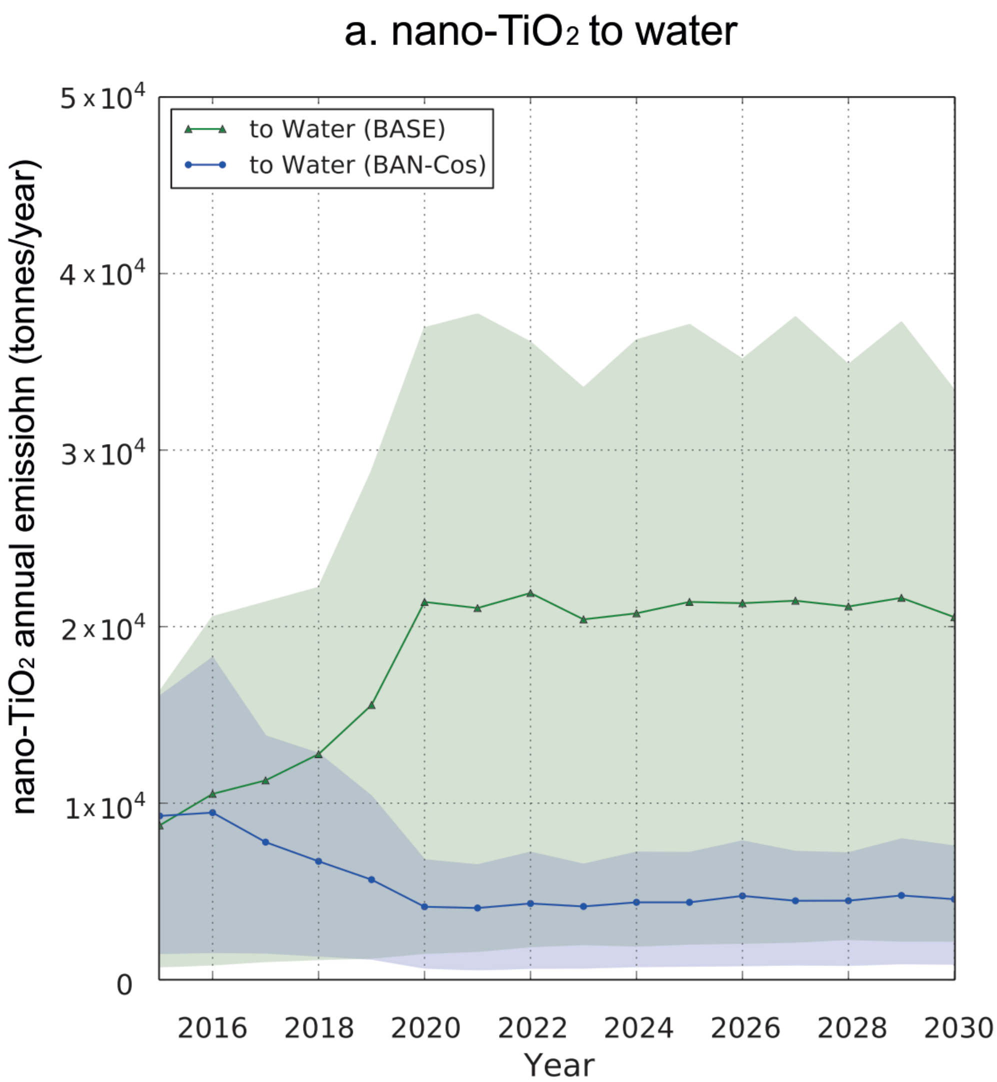
Scenario results



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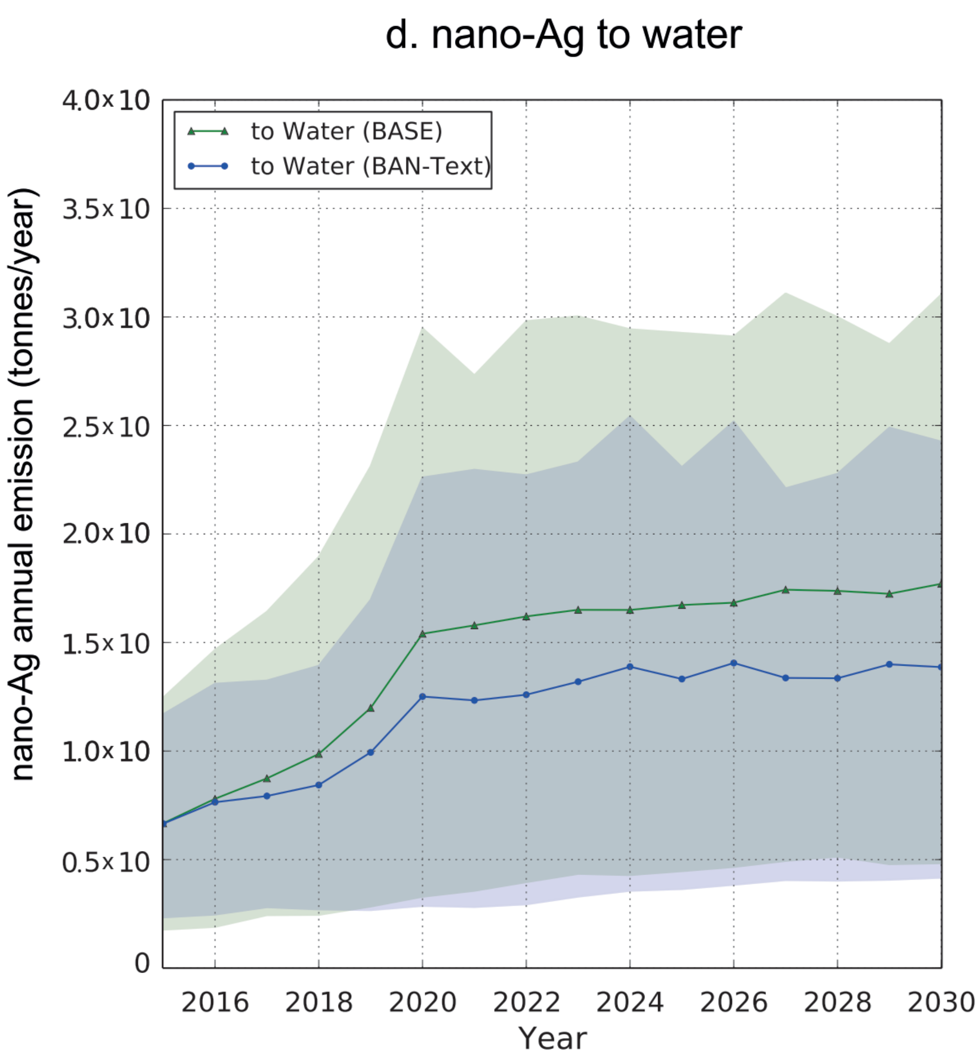

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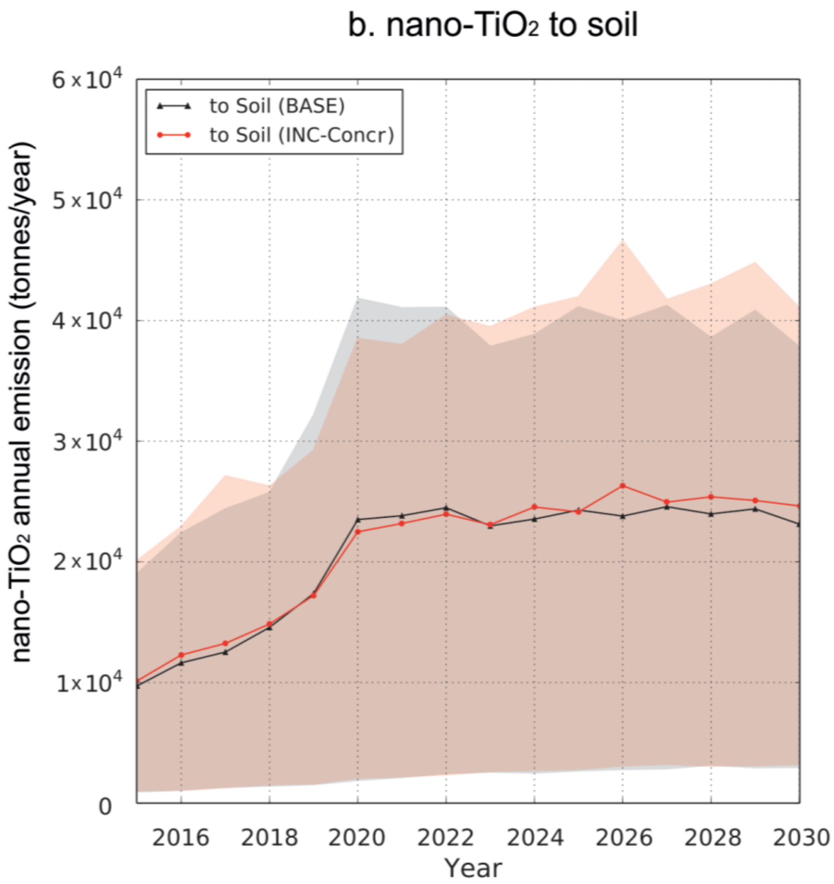

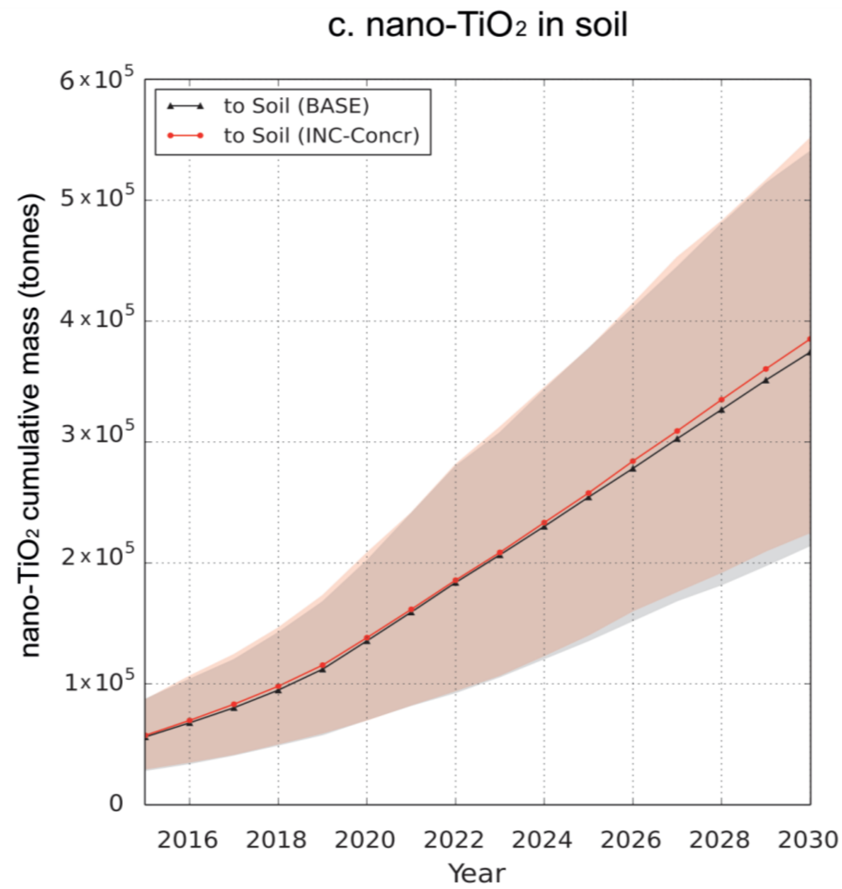

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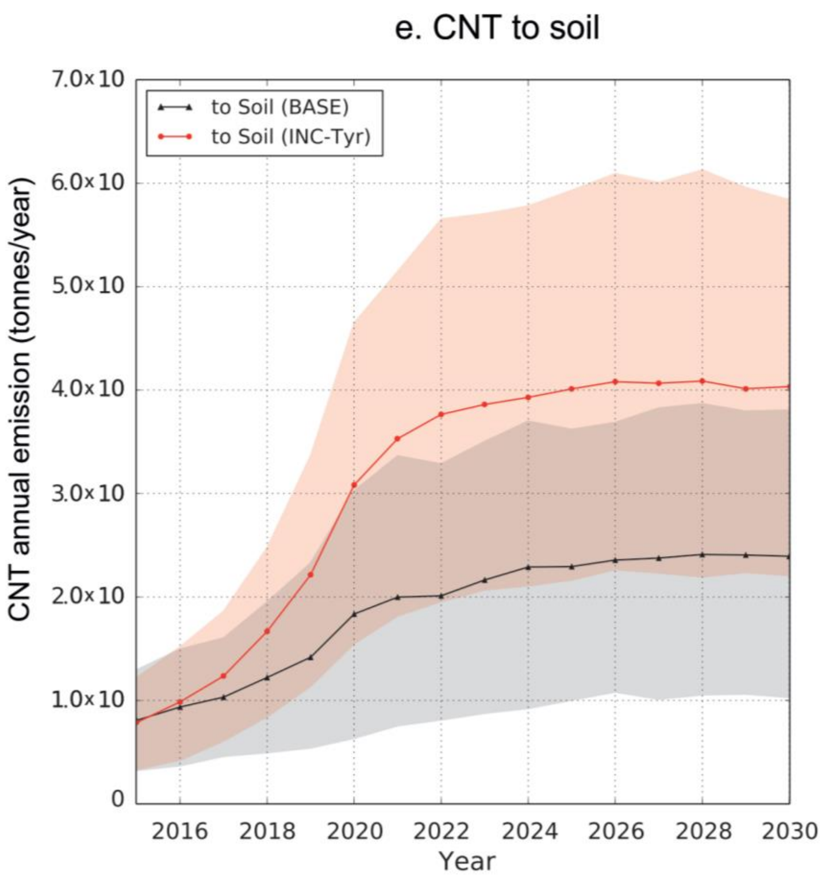

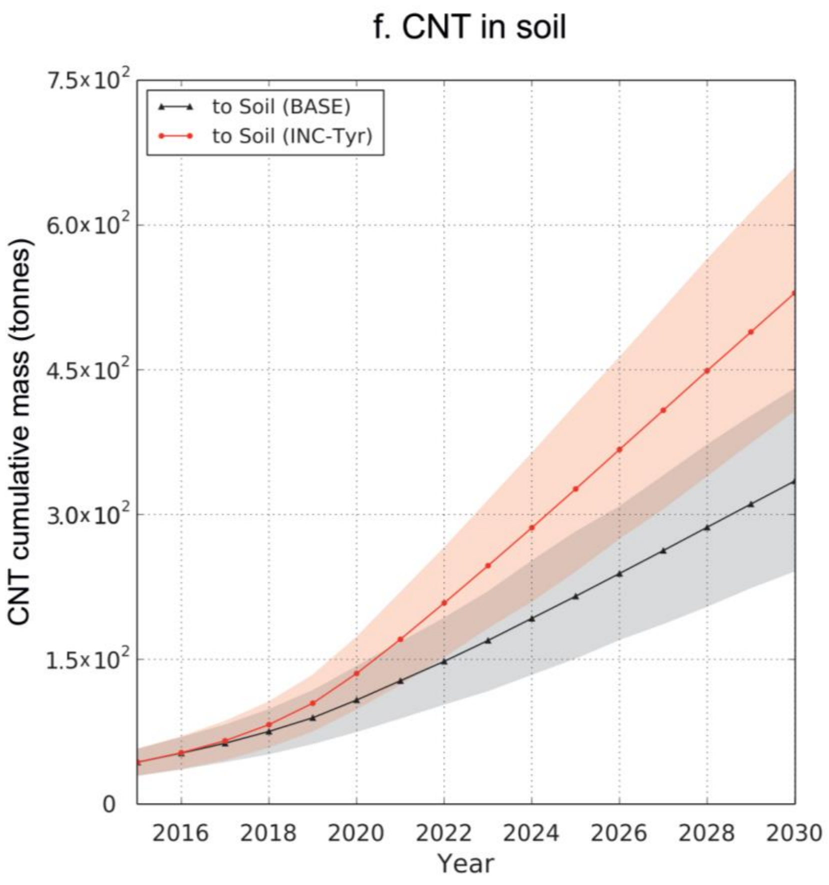

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Conclusions

- Material flow modeling is crucial for predicting flows of ENM to the environment
- Probabilistic MFA can incorporate the high uncertainty of many parameters, mainly production and product use
- Dynamic MFA is able to calculate amounts in stocks and sinks
- Detailed flow models for many ENM available
  - realistic
  - prospective
  - dynamic

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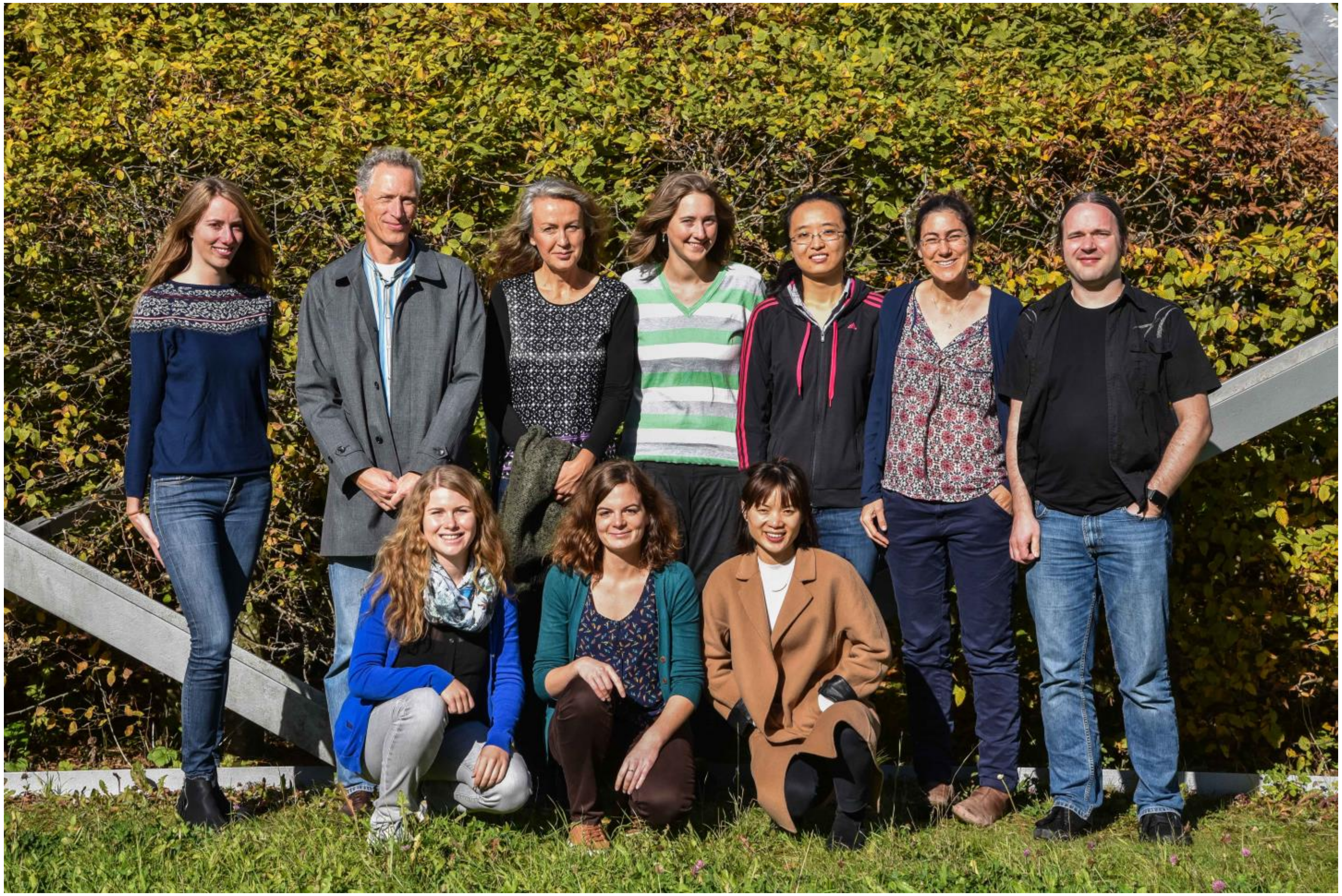
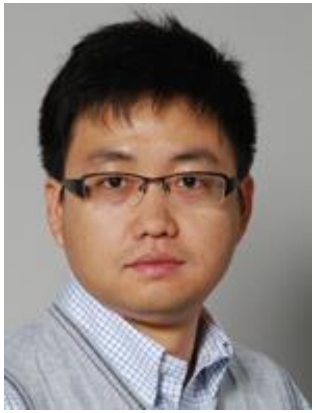
Acknowledgements



Nikolaus Bornhöft



Tianyin Sun

Opportunities and Risks of Nanomaterials
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MARINA
MANAGING RISKS OF NANOMATERIALS

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