Modelling of *releases* of nanoparticles into the environment

Bernd Giese

ISR – Institut für Sicherheits- und Risikoforschung,

Univ. f. Bodenkultur Wien
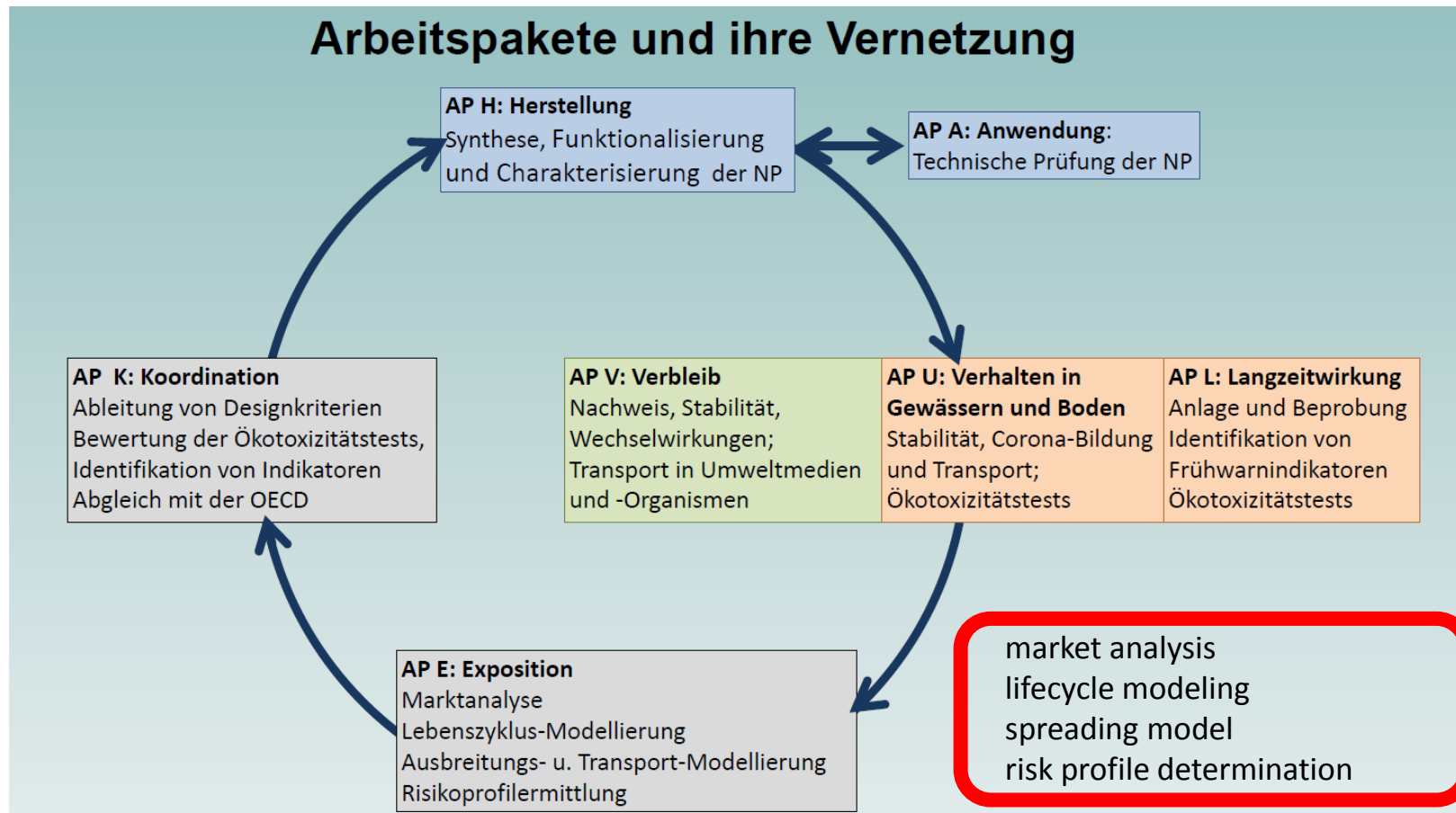
(vorm. Univ. Bremen)

Michael Steinfeldt (Uni Bremen)

Fadri Gottschalk

ETSS AG – Engineering, technical and scientific services

www.etss.ch

The BMBF project DENANA - Design Criteria for Sustainable Nanomaterials

Arbeitspakete und ihre Vernetzung

AP H: Herstellung
Synthese, Funktionalisierung und Charakterisierung der NP

AP A: Anwendung:
Technische Prüfung der NP

AP K: Koordination
Ableitung von Designkriterien
Bewertung der Ökotoxizitätstests,
Identifikation von Indikatoren
Abgleich mit der OECD

AP V: Verbleib
Nachweis, Stabilität,
Wechselwirkungen;
Transport in Umweltmedien
und -Organismen

AP U: Verhalten in Gewässern und Boden
Stabilität, Corona-Bildung und Transport;
Ökotoxizitätstests

AP L: Langzeitwirkung
Anlage und Beprobung
Identifikation von
Frühwarnindikatoren
Ökotoxizitätstests

AP E: Exposition
Marktanalyse
Lebenszyklus-Modellierung
Ausbreitungs- u. Transport-Modellierung
Risikoprofilermittlung

market analysis
lifecycle modeling
spreading model
risk profile determination

Data base of the modeling

- **Manufacturer of ENM**
  - Number, production volumes
  - Import and export volumes

- **ENM processing**
  - Product Categories
  - ENM consumption, ENM losses (+ emission paths)
  - Export and import of ENM-containing products

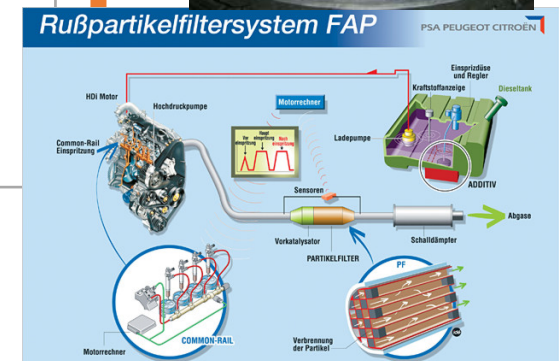- **Utilization** of ENM-containing products as well as emissions during application

- **Disposal** (regional resolution)
  - Sewage treatment (+ fraction for transfer to sewage sludge)
  - Landfill (+ transition to waste water, water, ground water)
  - Waste incineration (+ content in slag / ash)
  - Direct entry into air, water, soils
  - Recycling (+ share in recycled products)

  - **Conversion** into other compounds / forms during and after the utilization phase (e.g., formation of Ce_2S_3 in sewage sludge)
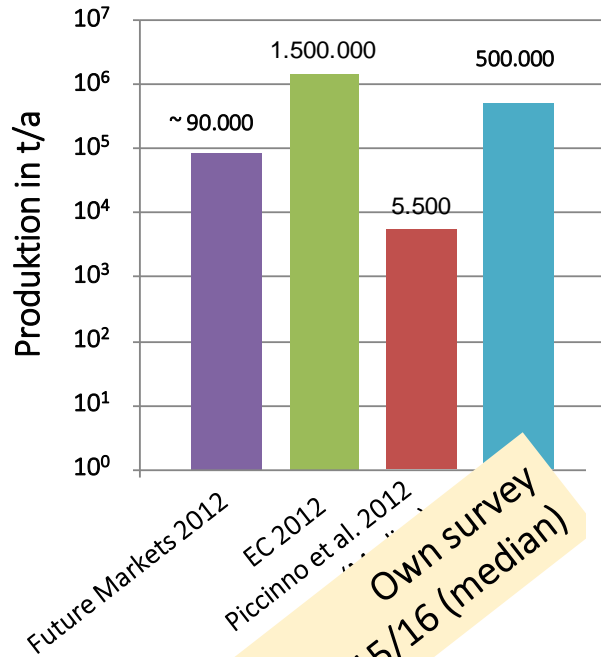
Product Use for SiO_2, CeO_2, and Ag-ENM

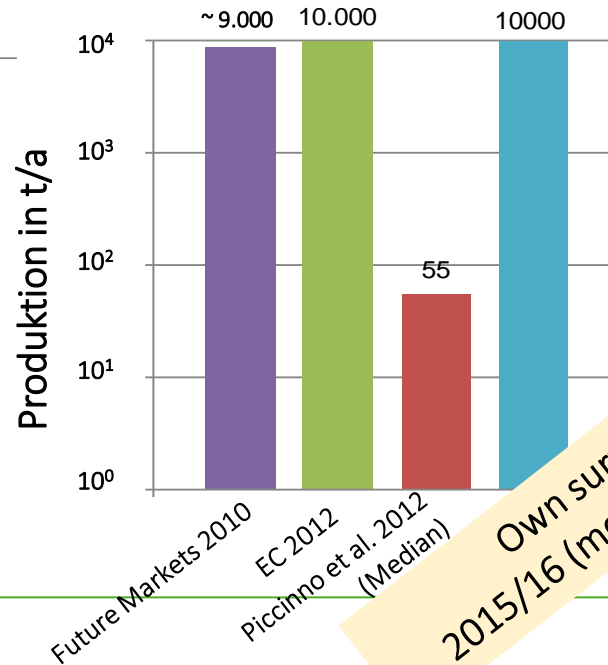| ENP-Typ	Produktkategorien
SiO_2	Coatings, textiles, building materials, polyesters, epoxy resins, adhesives, sealants, putty, lubricants
	Cosmetics, toothpaste, foodstuffs, medicines, ...
	Plastics, elastomers (silicone elastomers, tires, soles)
	Colors, inks
	support material
	Absorption and drying agents
CeO_2	Catalyst material
	Fuel additive (catalyst)
	Varnishes and coatings
	Polishing agents for glass and silicon wafers
	Nickel metal hydride (NiMH) batteries
Ag	Coating, plastics
	Detergents, filters, spray, cosmetics, medicine, foodstuffs
	Entertainment electronics, Computers
	textiles

Rußpartikelfiltersystem FAP   PSA PEUGEOT CITROËN

Production volumes international

SiO$_2$-ENP

Produktion in t/a

~ 90.000 · 1.500.000 · 5.500 · 500.000

Future Markets 2012 · EC 2012 · Piccinno et al. 2012 · Own survey 2015/16 (median)

CeO$_2$-ENP
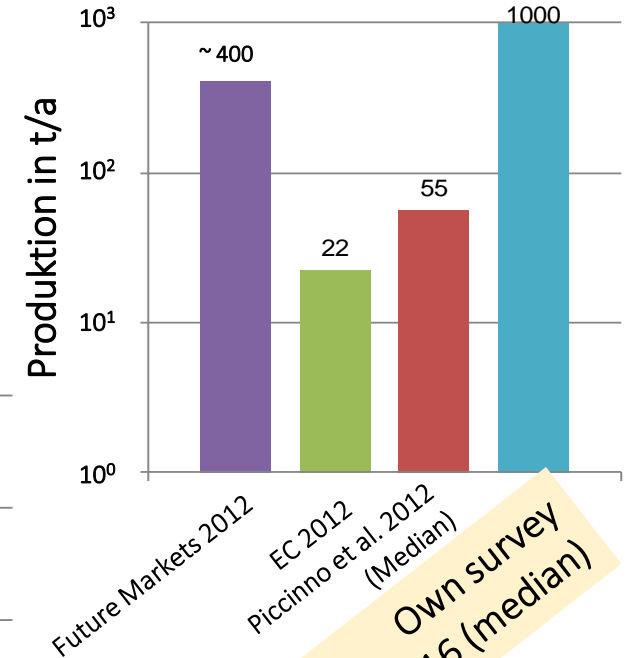
Produktion in t/a

~ 9.000 · 10.000 · 55 · 10000

Future Markets 2010 · EC 2012 · Piccinno et al. 2012 (Median) · Own survey 2015/16 (median)

Ag-ENP

Produktion in t/a

~ 400 · 22 · 55 · 1000

Future Markets 2012 · EC 2012 · Piccinno et al. 2012 (Median) · Own survey 2015/16 (median)

Silica-Type

Silica
7631-86-9

Synthetic amorphous silica
7631-86-9

Amorphous silica
7631-86-9

Crystalline silica
7631-86-9

Wet

Thermal

Surface treated silica (a)
67762-90-7
68611-44-9
68909-20-6

Natural

By-products

Cristobalite
14464-46-1

Silica gel
112926-00-8

Pyrogenic silica (b)
112945-52-5

Precipitated silica
112926-00-8

Figure 7: Theoretical SAS particles at infinite dilution

(a)

(b)

(c)

(d)

(a) Sol, isolated primary particles
(b) Gel, densified aggregate
(c) Precipitated, compact aggregates
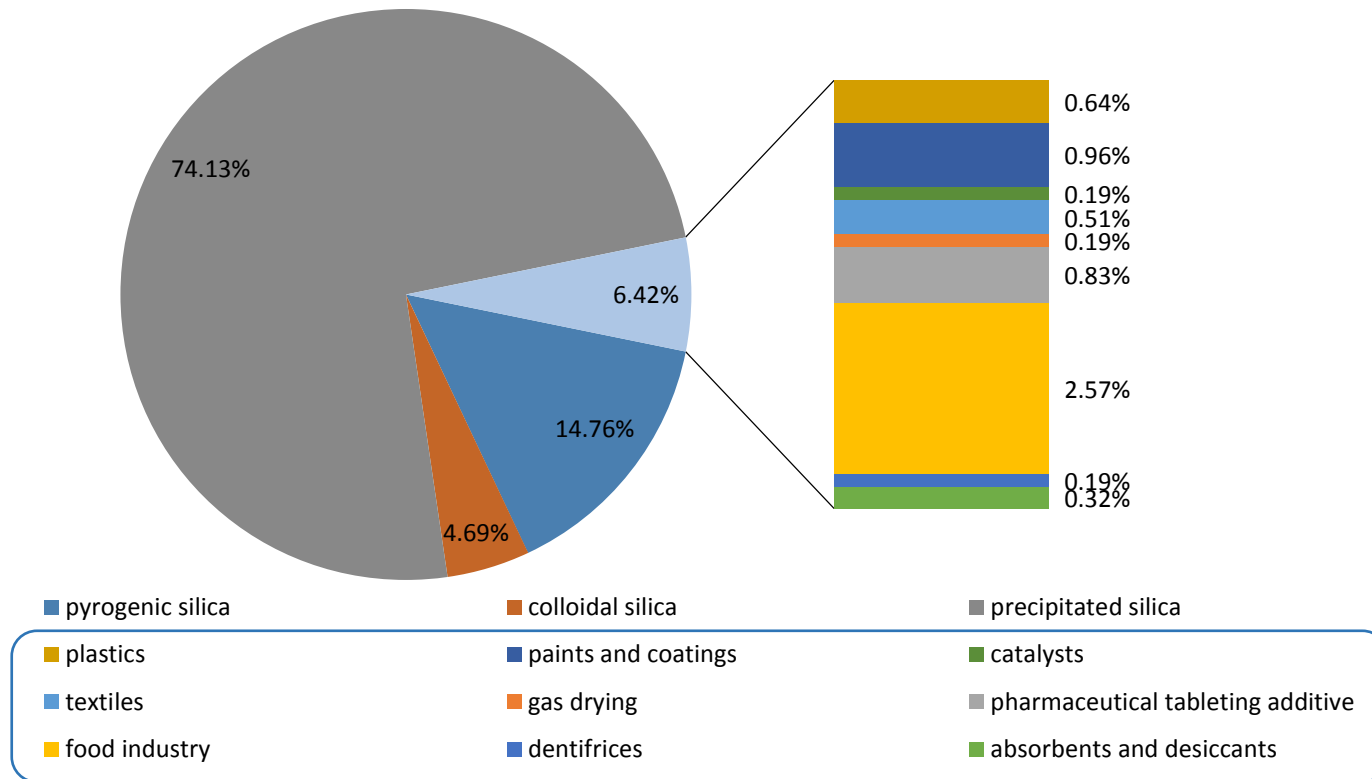(d) Pyrogenic, open branched-chain aggregates
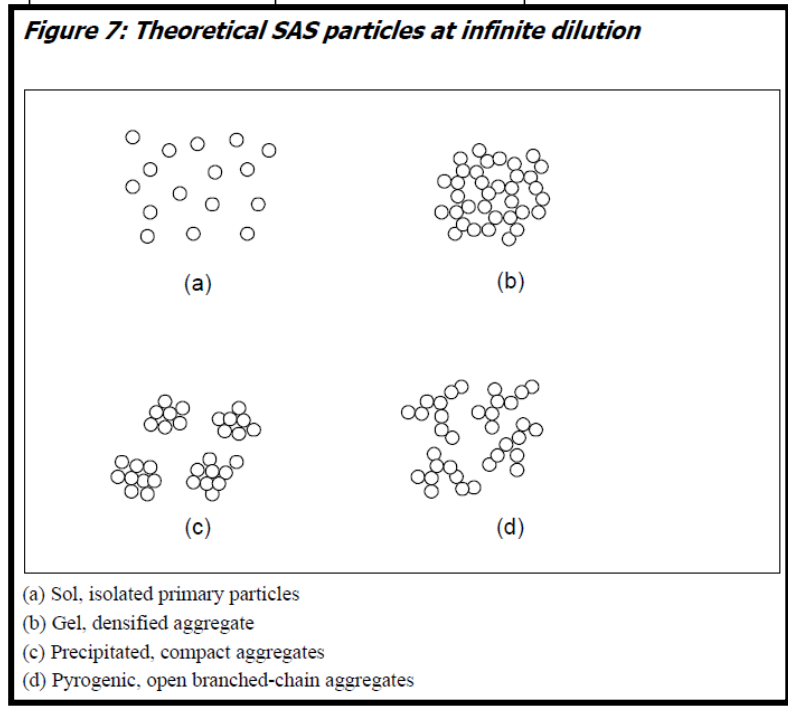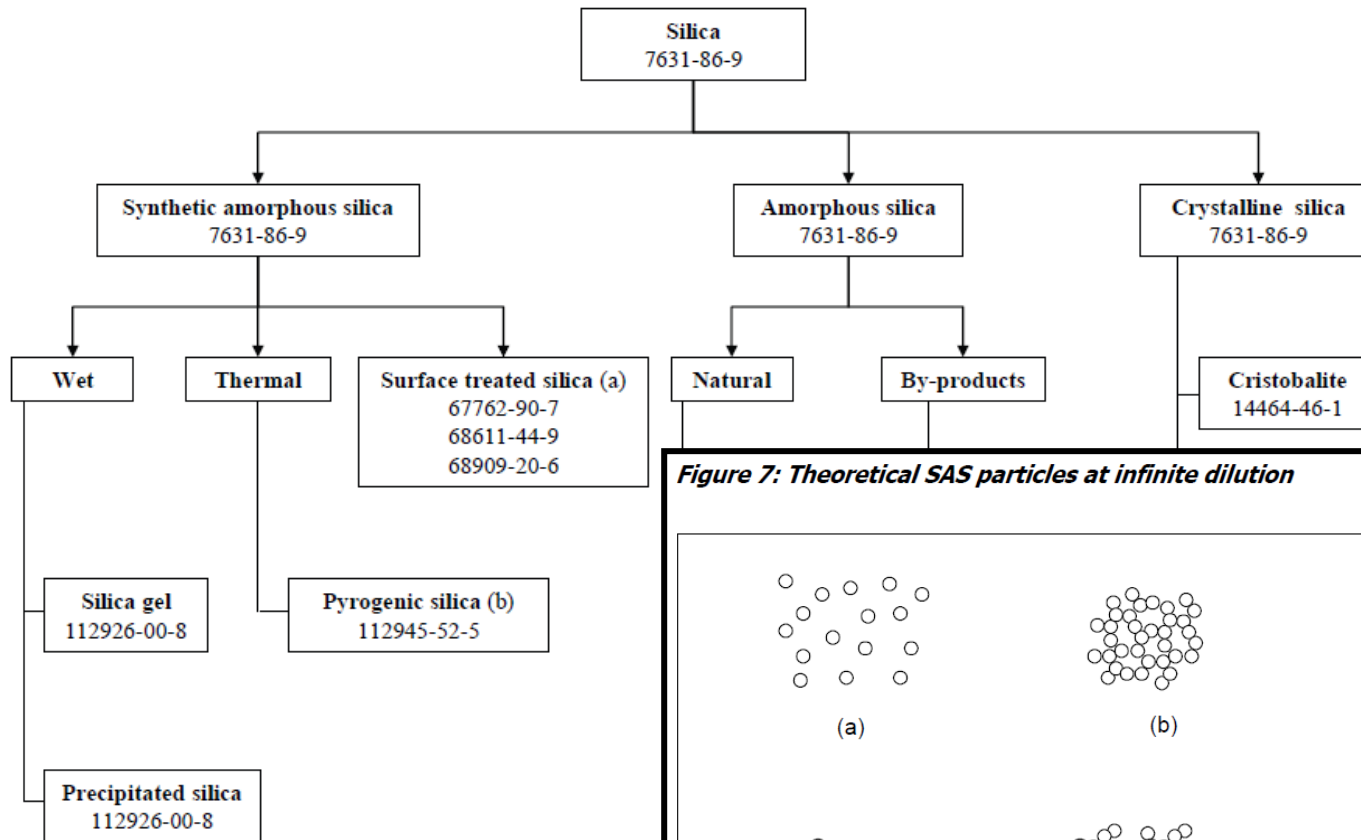
Source:
ECETOC JACC REPORT
No. 51 "Synthetic
Amorphous Silica"
Brussels, 2006

Precipitated SiO$_2$
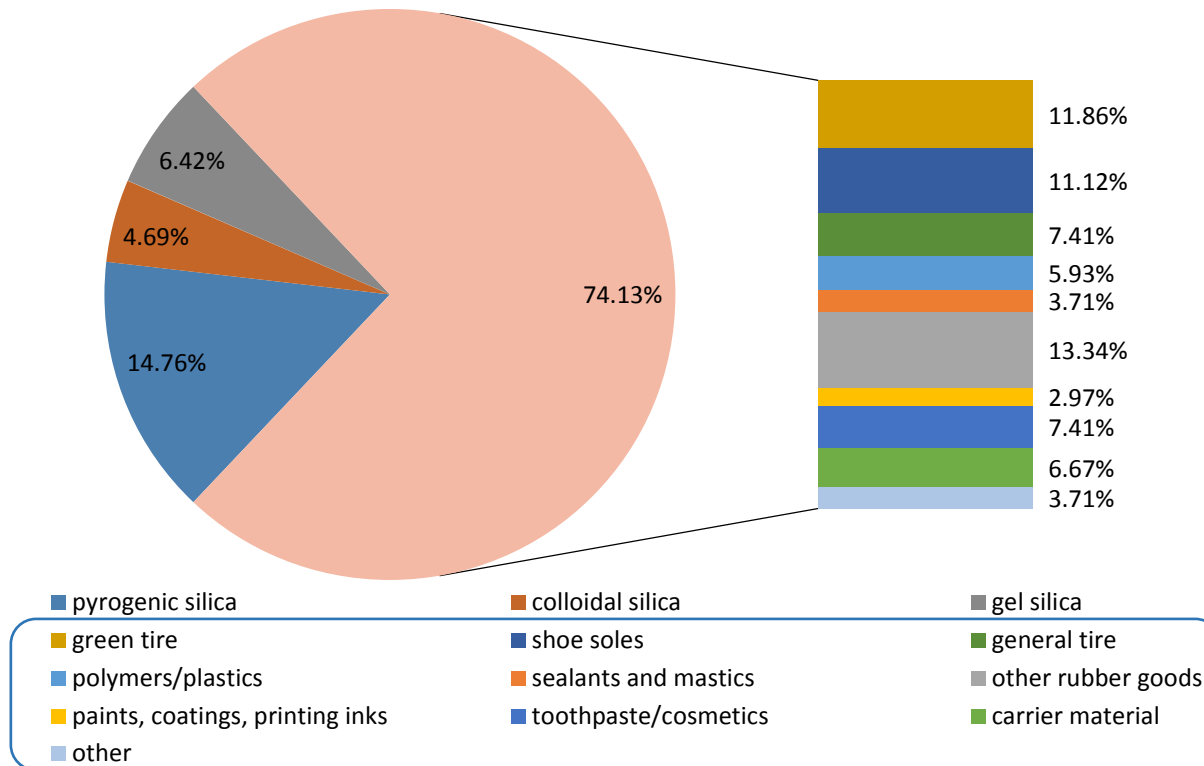
Aufteilung nach:Joint Assessment of Commodity Chemicals (JACC) – Report (2006) des European Centre for Ecotoxicology and Toxicology of Chemicals on Synthetic Amorphous Silica

SiO₂-gel

Aufteilung nach:Joint Assessment of Commodity Chemicals (JACC) – Report (2006) des European Centre for Ecotoxicology and Toxicology of Chemicals on Synthetic Amorphous Silica

6 Life cycle driven release and material state/location models developed:

A) Release

1) Life cycle release during product use (including delay due to use phase)
2) End of life release (EOL) (including delay due to non-release use phases)

B) Delay

3) Life cycle release delay during non-release use time periods
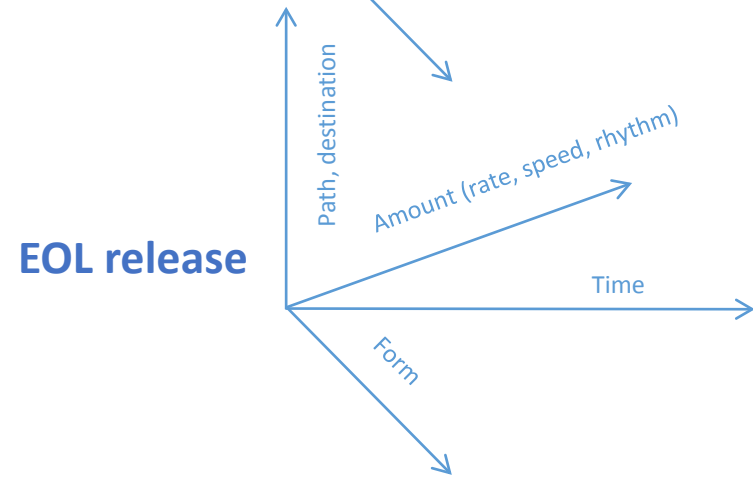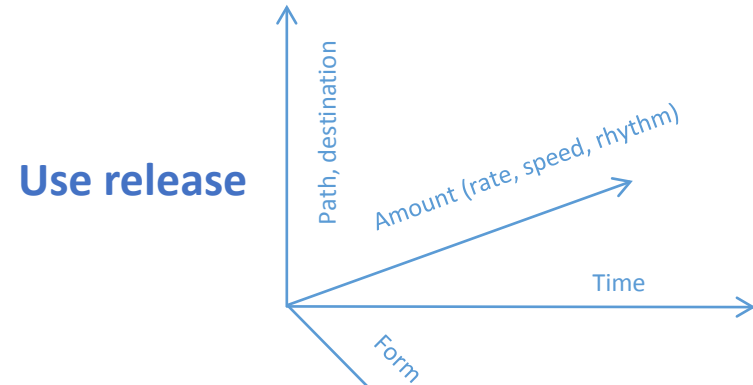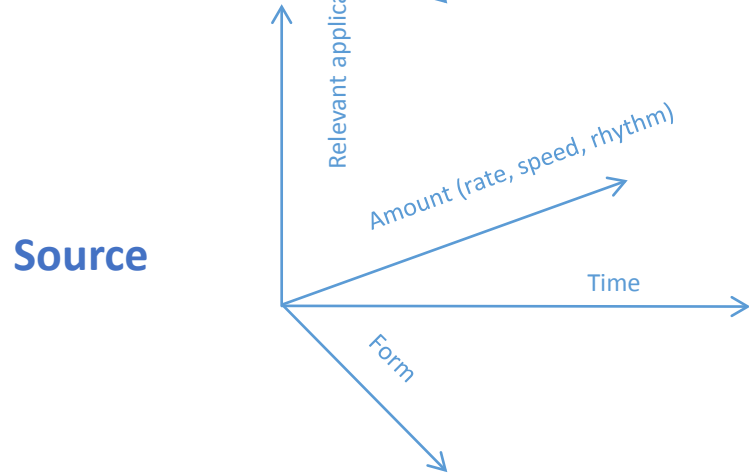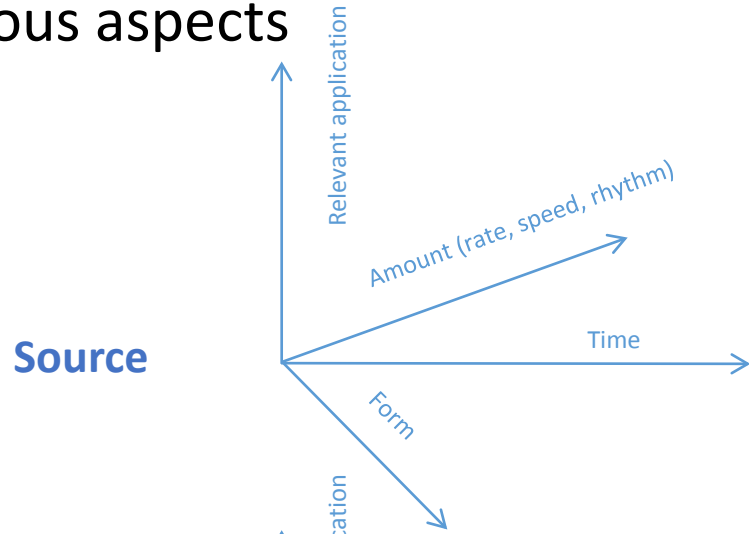4) EOL-Release delay in pre-EOL pahases

Out there

5) Already out there (nature) from product use sources
6) Already out there (nature) from product EOL sources

For the basic methods used, see:

Walser und Gottschalk,
Journal of Cleaner Production 80 (2014) 241e251
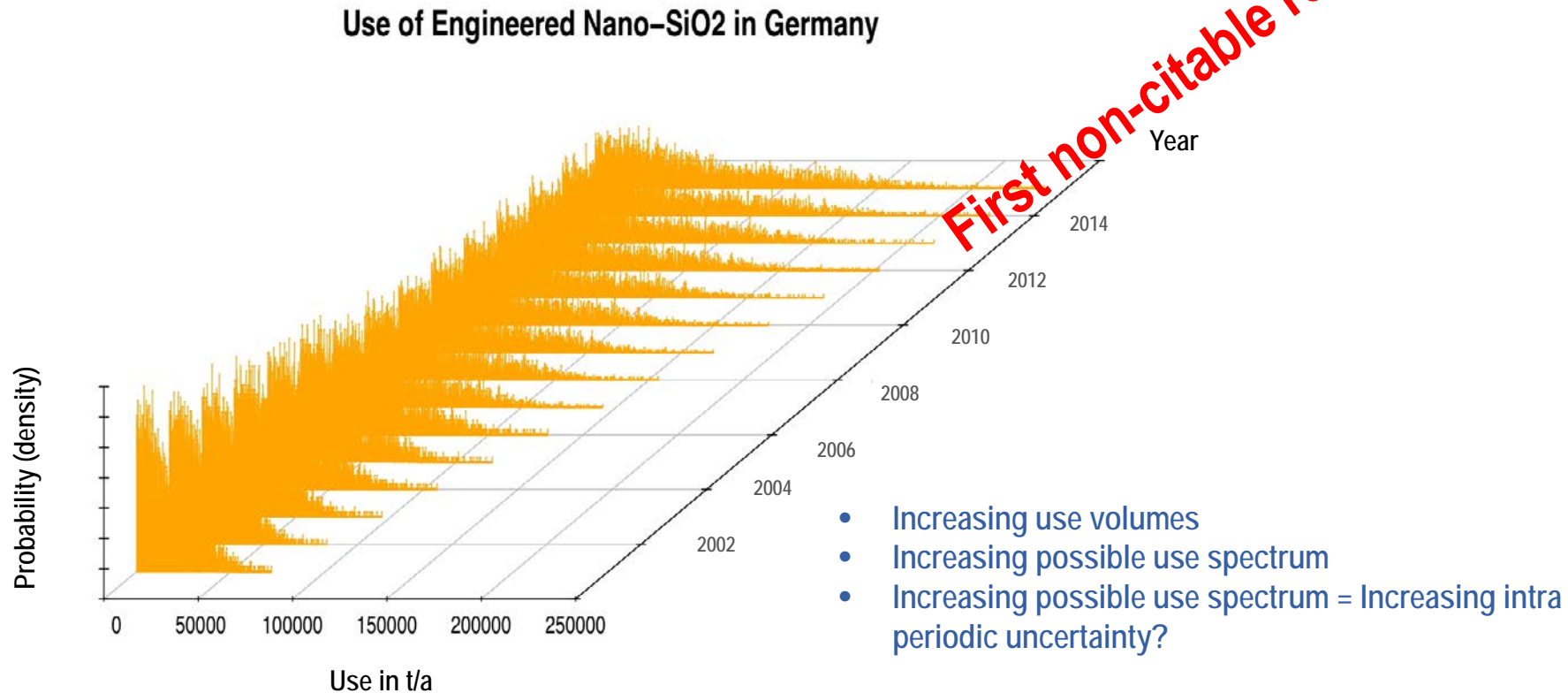http://dx.doi.org/10.1016/j.jclepro.2014.05.085

Life cycle models developed cont.

Dealing with distinct uncertainty/variability on various aspects

Life cycle models developed cont.
Challenges on stochastic production/use modeling

Use of Engineered Nano–SiO2 in Germany

First non-citable results.

- Increasing use volumes
- Increasing possible use spectrum
- Increasing possible use spectrum = Increasing intra periodic uncertainty?

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BOKU
ISR
Institut für Sicherheits-
und Risikowissenschaften
Universität für Bodenkultur Wien

Development of Probability Distribution

Total release of CeO_2-ENM:

First non-citable results.

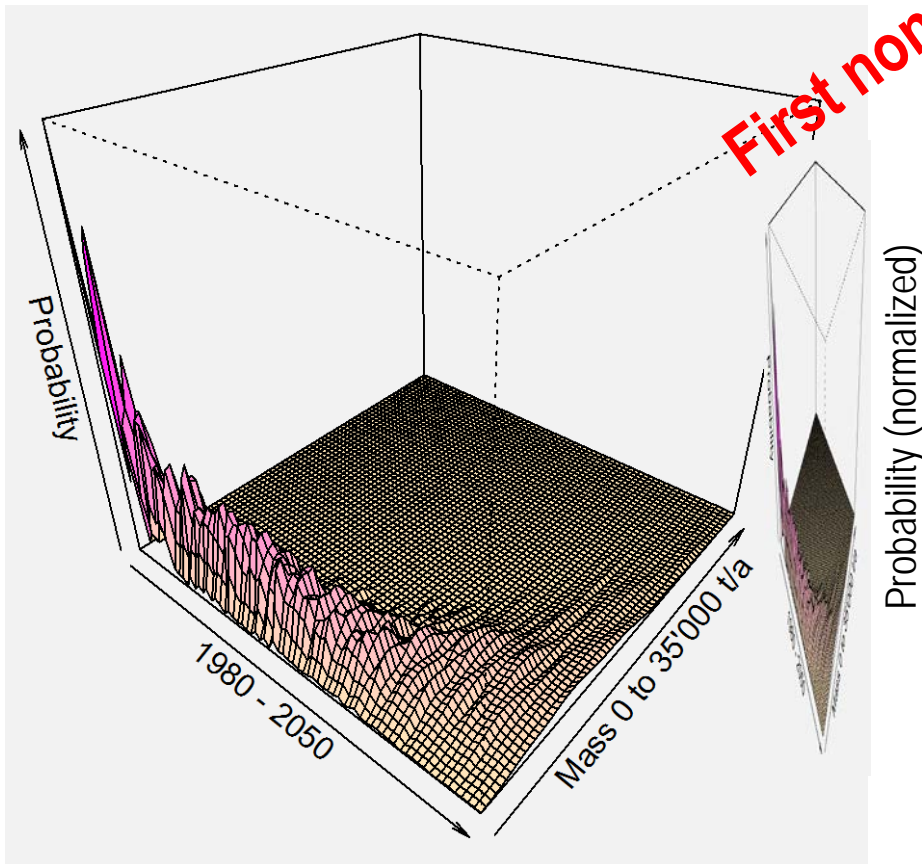| Use category	Share in %	Application start
Catalytic converters	28,3	1980
Fuel additive	0,1	2000
Exterior colors (among others wood)	0,5	2000
Polishes for glass and silicon wafers	51,9	1990
NiMH batteries	16,9	1990
automotive NiMH-batteries	2,3	2000
Further and unspecified categories with no relevant environmental	no data available	

For the basic method used, see:

Walser und Gottschalk,
Journal of Cleaner Production 80 (2014) 241e251
http://dx.doi.org/10.1016/j.jclepro.2014.05.085

Development of Probability Distribution

CeO2-ENM from use release :

Use category	Share in %	Application start
Catalytic converters	28,3	1980
Fuel additive	0,1	2000
Exterior colors (among others wood)	0,5	2000
Polishes for glass and silicon wafers	51,9	1990
NiMH batteries	16,9	1990
automotive NiMH-batteries	2,3	2000
Further and unspecified categories with no relevant environmental	no data available	

First non-citable results.

Mass distribution of the total release SiO$_2$-ENM

Release into Nature

First results (non-citable).

2000

2020

2050

Mass in t/a

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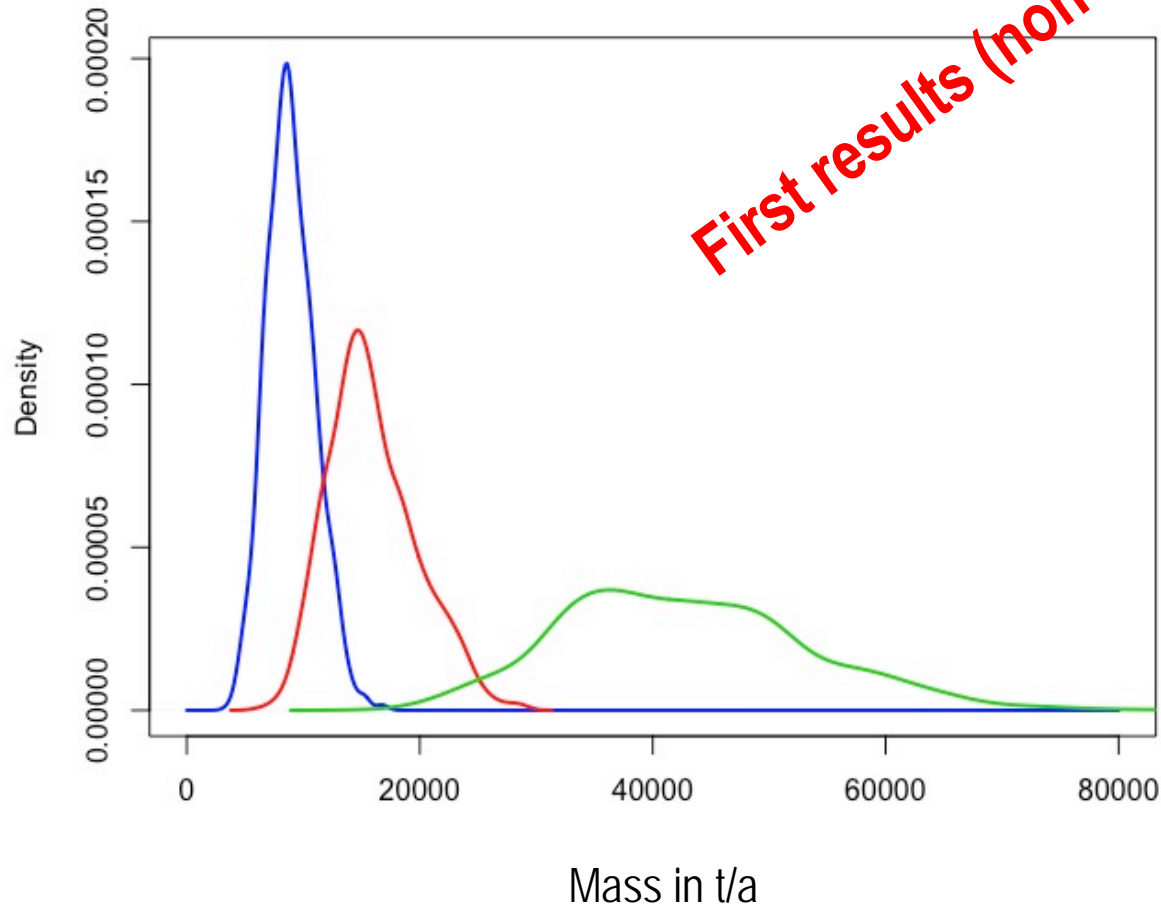
Mass distribution of the total release in 2017 CeO$_2$-ENM

Universität für Bodenkultur Wien

Institut für Sicherheits- und Risikowissenschaften

First results (non-citable)

Release into Nature
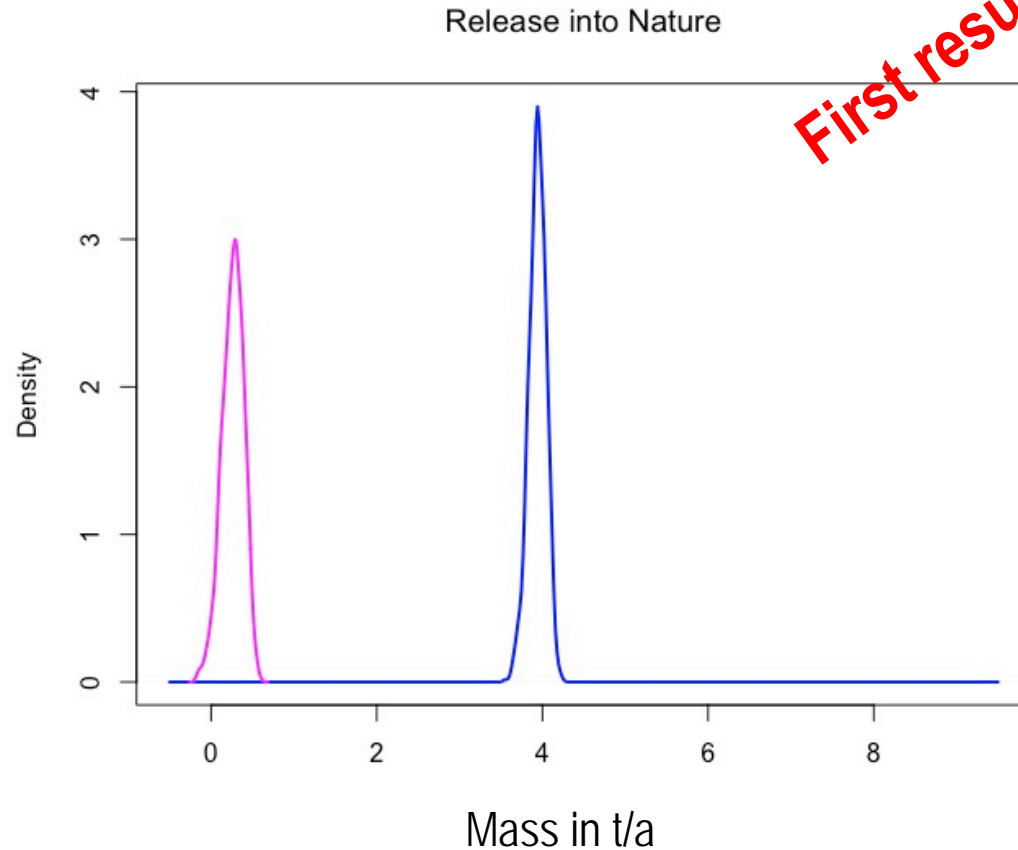
Use-release

EOL-release

Preliminary findings

- Dynamic modeling is possible with existing data

- Increasing uncertainties in quantity, temporal and spatial dimension (type of compartments)

- Statements on the potential concentration distribution are nevertheless possible

- (Up to now) results partially correspond to previous predictions

What would be helpful in the future:

- Information on the production volume of the ENM and the degree of dissemination of the corresponding technologies (for example number of vehicles equipped)

- Independent determination of real, application-related emissions

Contact

contact@etss.ch
Fadri Gottschalk
ETSS AG
www.etss.ch

Chaflur 136B
CH- 7558 Strada
Schweiz
Tel. +41(0)81 860 10 85

Fortunagasse 15
8001 Zürich, Schweiz

+41(0) 43 233 82 67

bernd.giese@boku.ac.at
Bernd Giese
Institut für Sicherheits- und
Risikowissenschaften (ISR)
Universität für Bodenkultur (BOKU)
Borkowskigasse 4
1190 Wien (Austria)

Tel. +43-1-47654-818 15