



Multidimensional Risk Analysis of Chemicals

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Transforming dangers into risks

- Society is **unconsciously** affected by many chemical substances
- Risks can be attributed to **conscious** decisions
- If there is no risk communication, there are no risks

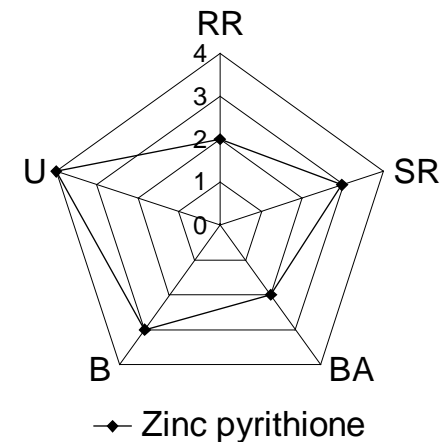


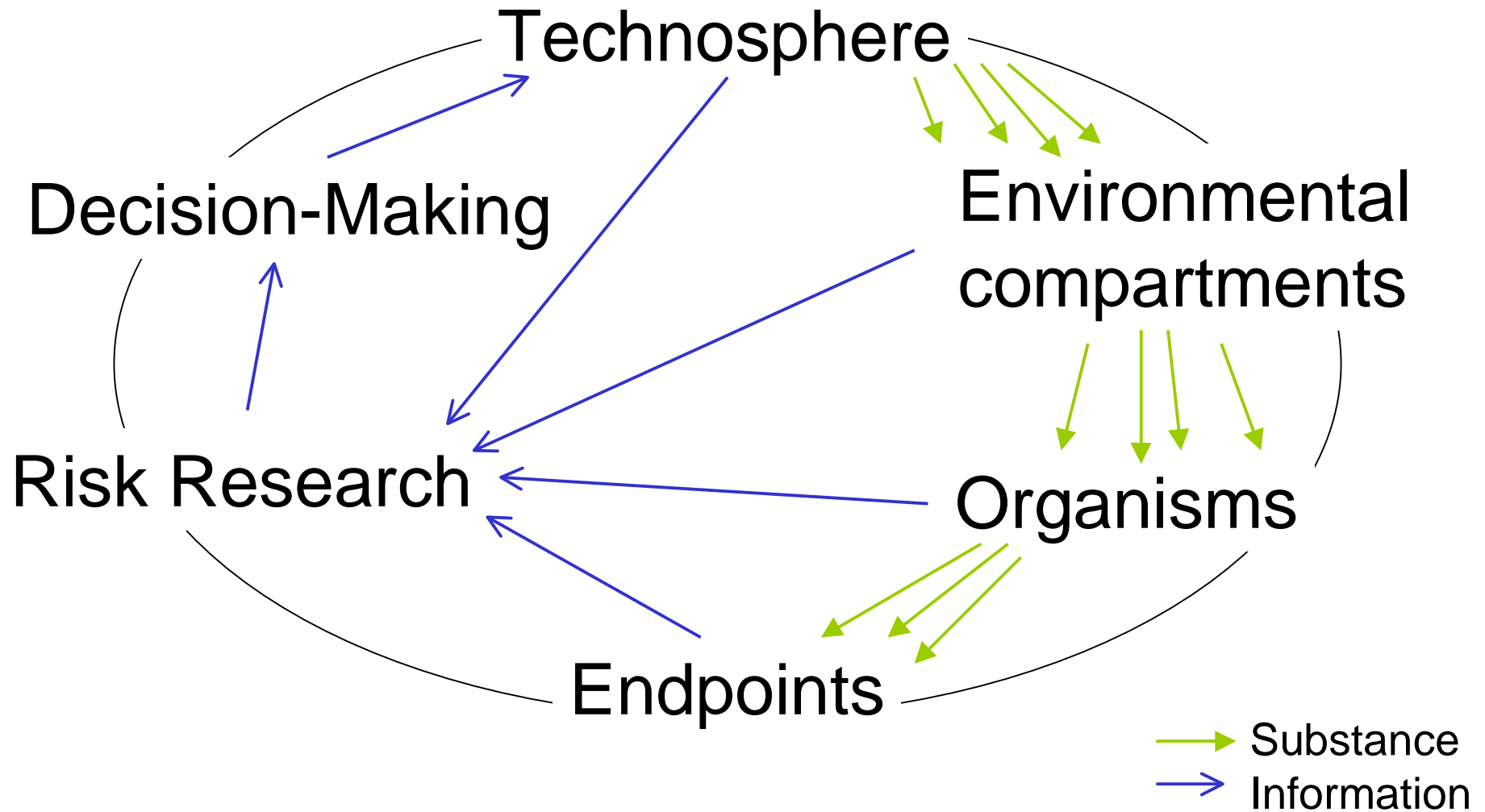
Why multidimensional?

- The risks of society are not a genuine scientific problem
- Science should have an opinion, but not try to completely determine decisions

PEC/PNEC?

Risk profile!







Indicators of Ecotoxicological risk

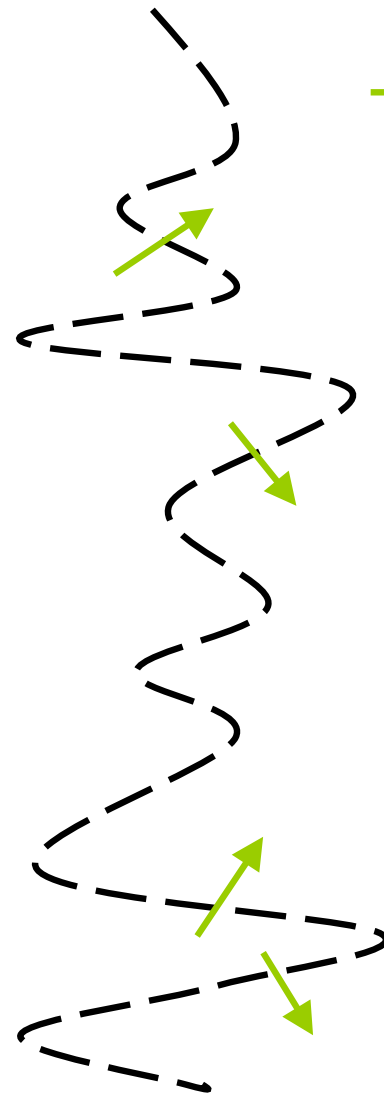
- Release
 - Data mining
- Spatiotemporal Range
 - Qualitative scoring (Scale 1 to 4)
- Bioaccumulation
 - Comparative risk profiles
- Biological Activity
- Uncertainty

Ranke J, Jastorff B (2000) *Environ Sci Poll Res* 7(2) 105-114



Release

→ Chemical discharge



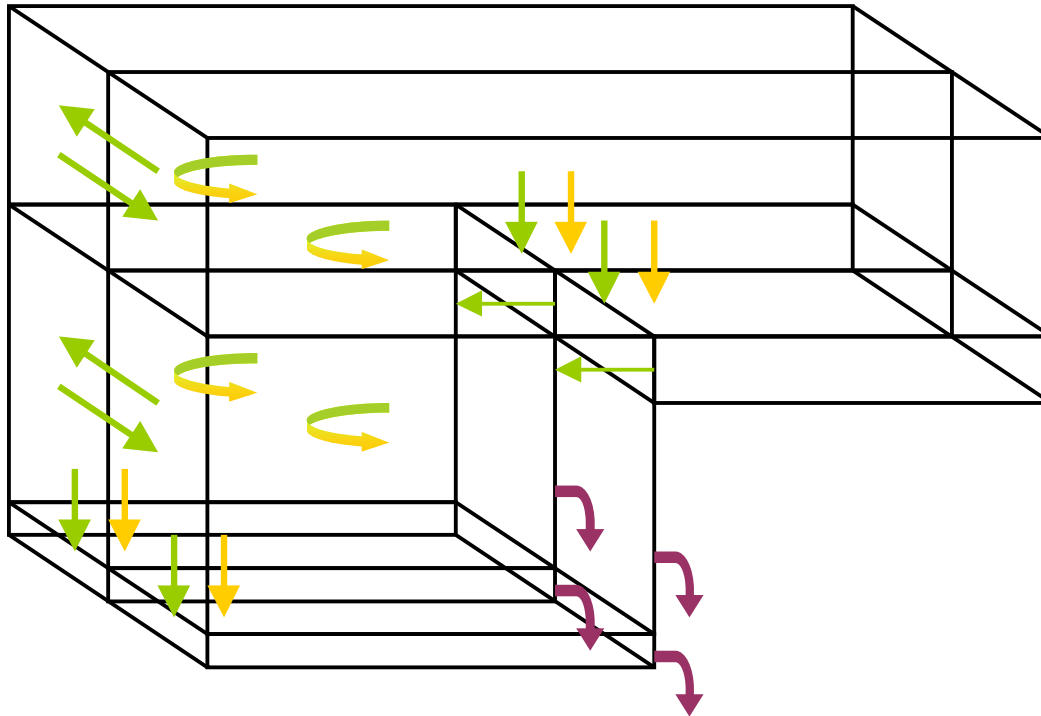
$$\begin{pmatrix} S_{1(t)} \\ S_{2(t)} \\ \dots \\ \dots \\ S_{n(t)} \end{pmatrix} \Rightarrow S_{tot}$$

Technosphere

Environment



Spatiotemporal range



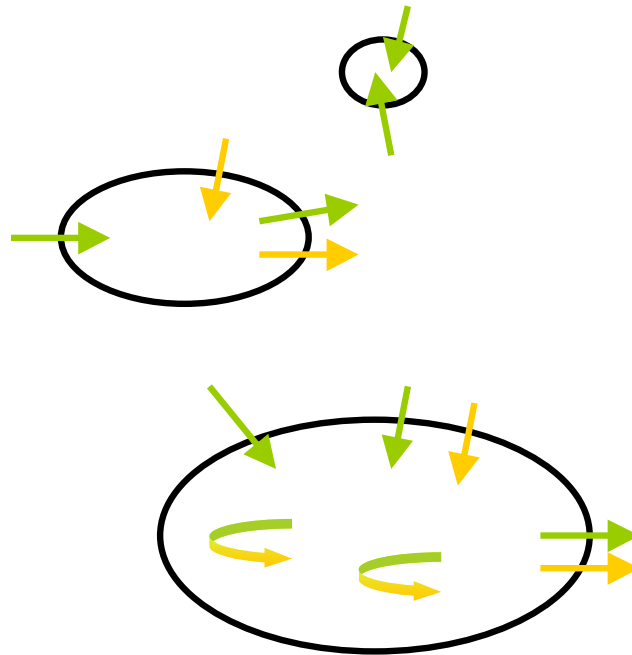
Environmental compartments

$$\begin{pmatrix} \mathbf{M}_{a(t)} \\ \mathbf{M}_{b(t)} \\ \dots \\ \dots \\ \mathbf{M}_{n(t)} \end{pmatrix} \Rightarrow \tau$$

 Transport
Reaction
Elimination



Bioaccumulation



$$\begin{pmatrix} \mathbf{B}_{1(t)} \\ \mathbf{B}_{2(t)} \\ \dots \\ \dots \\ \mathbf{B}_{n(t)} \end{pmatrix} \Rightarrow f_o$$

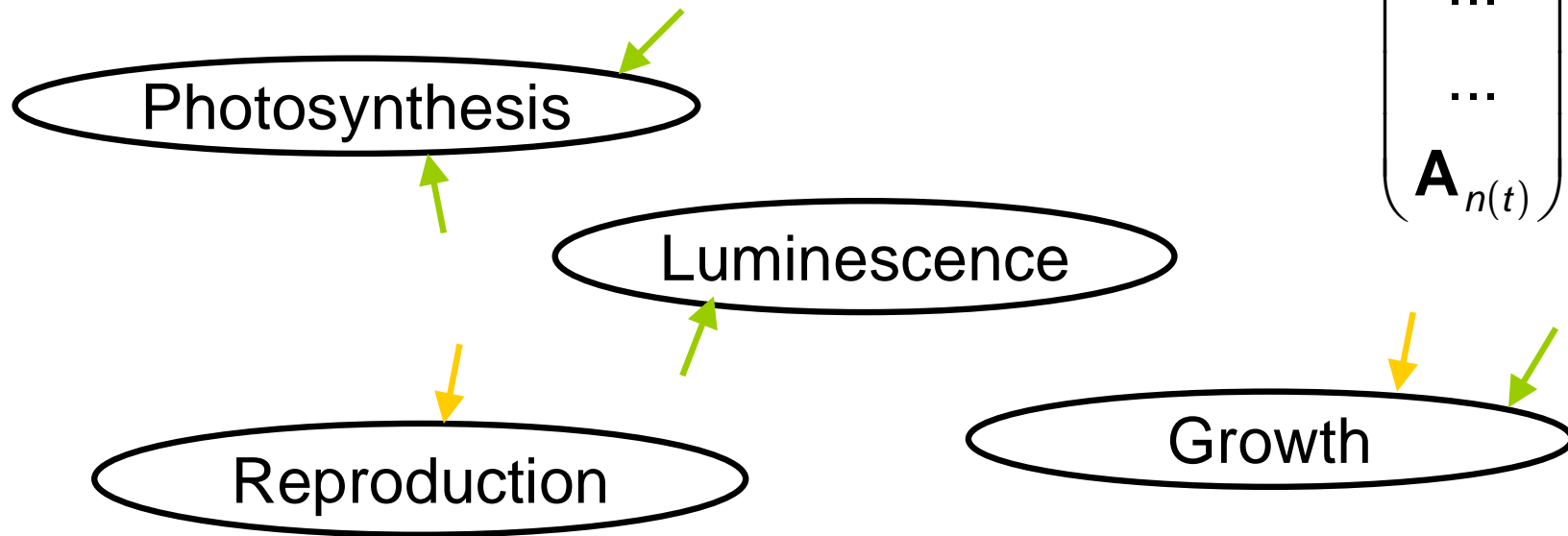
Organisms

- Chemical uptake/elimination
- ↻ Metabolic transformation
- Transformation product uptake/elimination



Biological Activity

$$\begin{pmatrix} \mathbf{A}_{1(t)} \\ \mathbf{A}_{2(t)} \\ \dots \\ \dots \\ \mathbf{A}_{n(t)} \end{pmatrix} \Rightarrow A$$



Endpoints

- Chemical effect
- Transformation product effect



Uncertainty

- Relative amount of data
- Ambiguity of data
- Adequacy of data

$$\begin{pmatrix} U_{S_{\text{tot}}} \\ U_{\tau} \\ U_{f_0} \\ U_A \end{pmatrix} \Rightarrow U$$

Risk Science



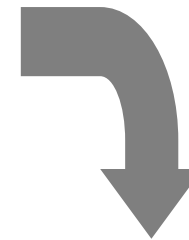
UFT_SAR - Netscape

Database UFT_SAR

SQL-query: select * from bioactivity where chent like "MercaptoBT"

pk	chent	organism	effect	route	exposition [g/g] or [g/L]	unit	c_var	type	time_obs	T	comment	eff_source	eff_N
2	MercaptoBT	Fungus, 15 different Candida strains	Growth inhibition		39.5 E-3	g/L	0.974	EC50	---	---	Comment	deweve97	13
3	MercaptoBT	Fungus, Aspergillus niger	Growth inhibition		33 E-3	g/L	---	EC100	5 d	---	Comment	deweve97	13
4	MercaptoBT	Soil bacteria community	Ammonia oxidation		3 E-3	g/L	---	EC100	---	---	Comment	deweve97	13
5	MercaptoBT	Soil bacteria community	Nitrit reduction		0.067 E-0	g/L	---	EC40	---	---	Comment	deweve97	13
6	MercaptoBT	Fungus, Microsporum gypsum	Growth inhibition		0.05 E-0	g/L	---	EC100	---	---	Comment	foltinova78	65
7	MercaptoBT	Fungus, Epidermophyton floccosum	Growth inhibition		0.05 E-0	g/L	---	EC100	---	---	Comment	foltinova78	65
8	MercaptoBT	Soil bacteria community	Ammonia oxidation		3 E-3	g/L	---	EC75	---	---	Comment	tomlinson66	146
9	MercaptoBT	Activated sludge bacteria community	Global nitrifying activity		5 E-3	g/L	---	EC74	---	---	Comment	tomlinson66	146
10	MercaptoBT	Bacteria, model sediment columns	Nitrification		0.2 E-3	g/L	---	EC50	---	---	Comment	deweve97	13
11	MercaptoBT	Bacteria, Staphylococcus aureus	Growth inhibition		42 E-3	g/L	---	EC50	---	---	Comment	foltinova78	65
12	MercaptoBT	Bacteria, Bacillus subtilis	Growth inhibition		42 E-3	g/L	---	EC50	---	---	Comment	foltinova78	65
13	MercaptoBT	Escherichia coli	Growth inhibition		42 E-3	g/L	---	EC50	---	---	Comment	foltinova78	65
14	MercaptoBT	Bacteria, Staphylococcus	Growth inhibition		0.135	g/L	---	EC100	---	---	Comment	foltinova78	65

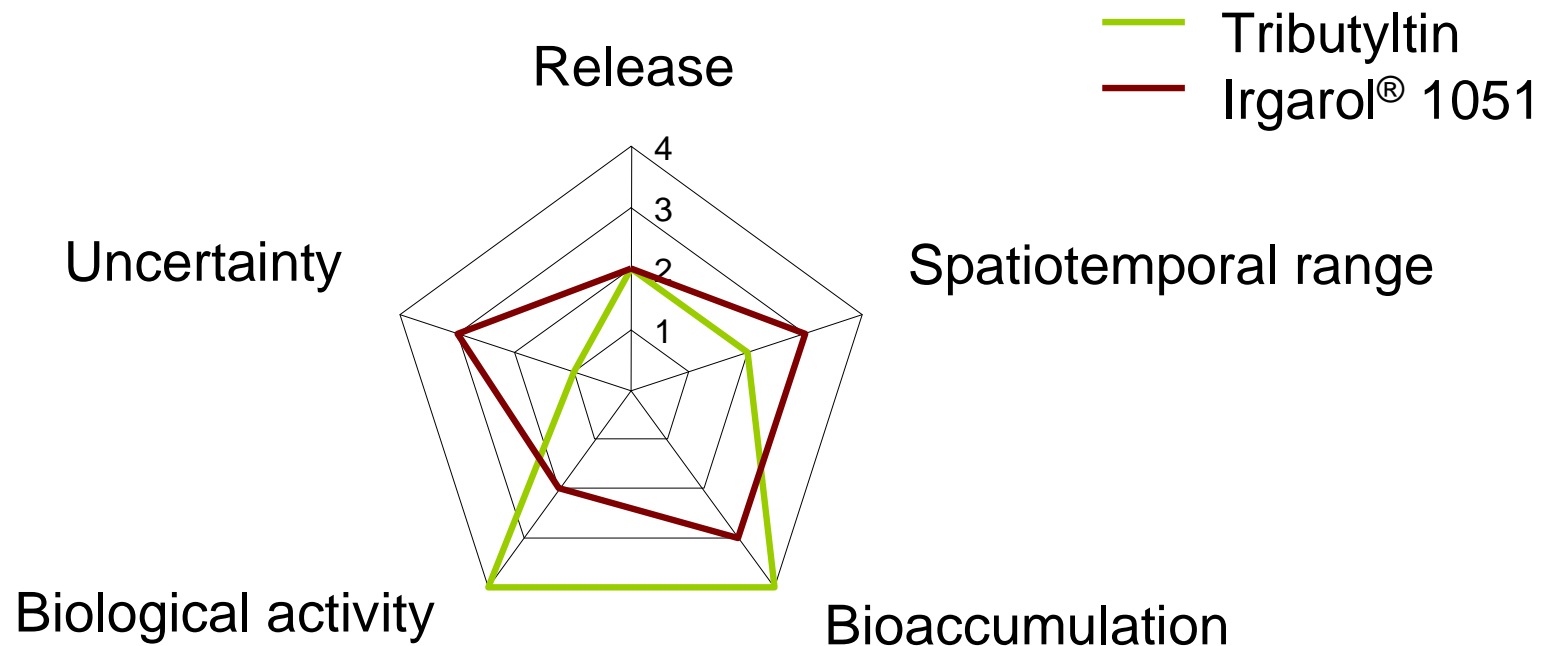
- Data collection
- Data processing
- Qualitative scoring



	Release	Range	Bioacc.	Activity	Uncertainty
Tributyltin	2 A	2 B	4 A	4 A	A
Irgarol® 1051	2 D	3 C	3 C	2 B	C



Risk profiles





Conclusions

- Each indicator score is disputable
- A differentiated comparison of substances is possible
- An improved risk consciousness will lead to improved risk management



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<http://www.uft.uni-bremen.de/chemie/ranke>