

# The use of fate models for the risk analysis of chemicals

## *Models and exposure based indicators*

Kolloquium Risikoforschung

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# Road map

1. Context of sustainable product design
2. Fate indicators
3. Spatiotemporal range
4. Model types and examples
5. Conclusions

# Fate and sustainability

- Intergenerational equity

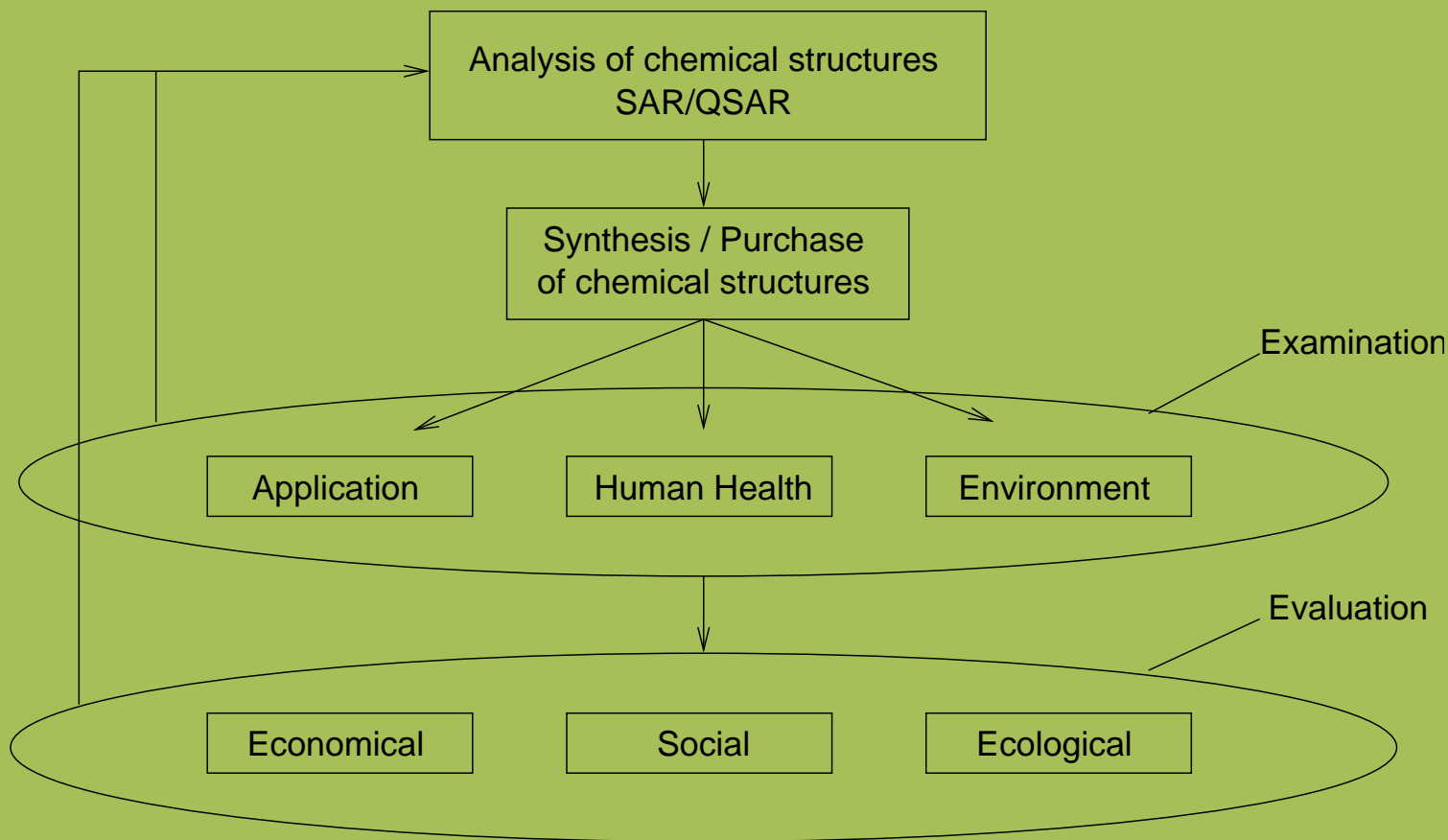
# Fate and sustainability

- Intergenerational equity
- Social justice

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- Intergenerational equity
- Social justice
- Ecosystem protection

# Sustainable Product Design



# Fate indicators

- Single-medium half life

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- Mobility
- Characteristic Travel Distance
- Spatial range

# Fate indicators

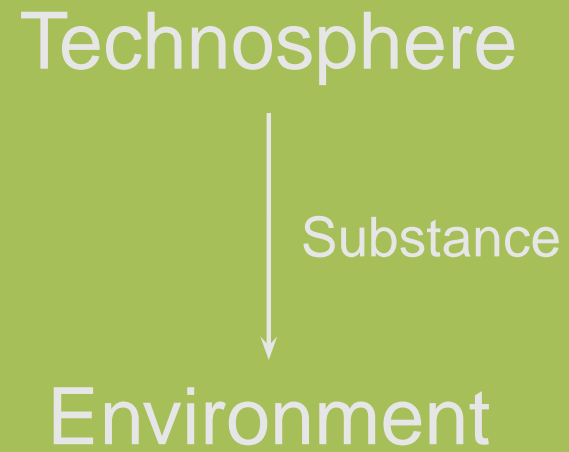
- Single-medium half life
- "Overall" persistence
- Henry constant, sorption constants
- Mobility
- Characteristic Travel Distance
- Spatial range
- Predicted Environmental Concentrations

# Using five risk indicators

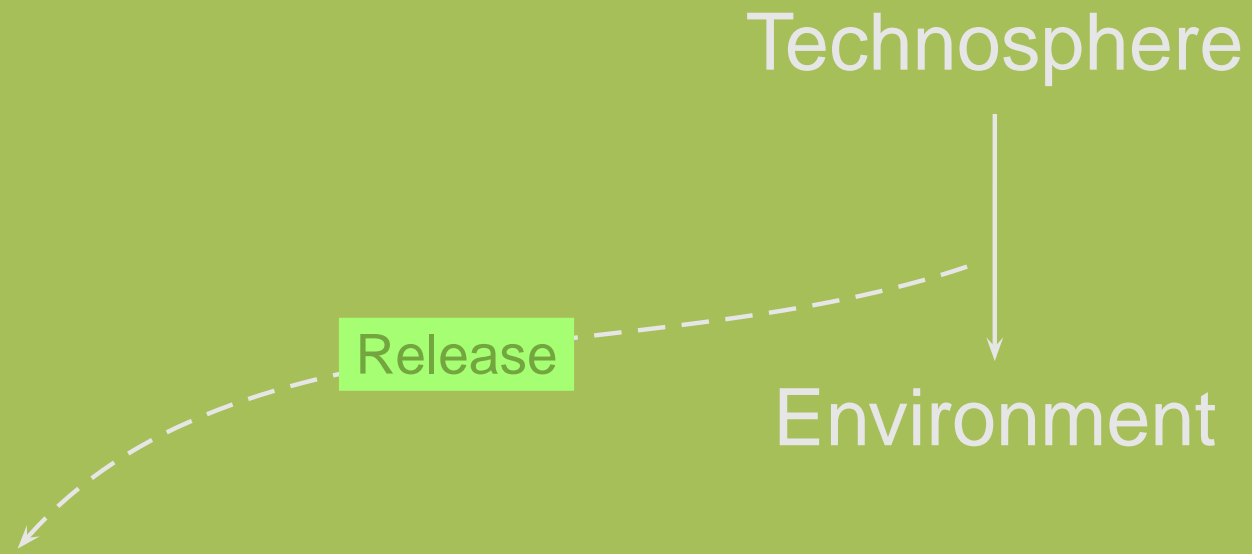
Technosphere

Environment

# Using five risk indicators



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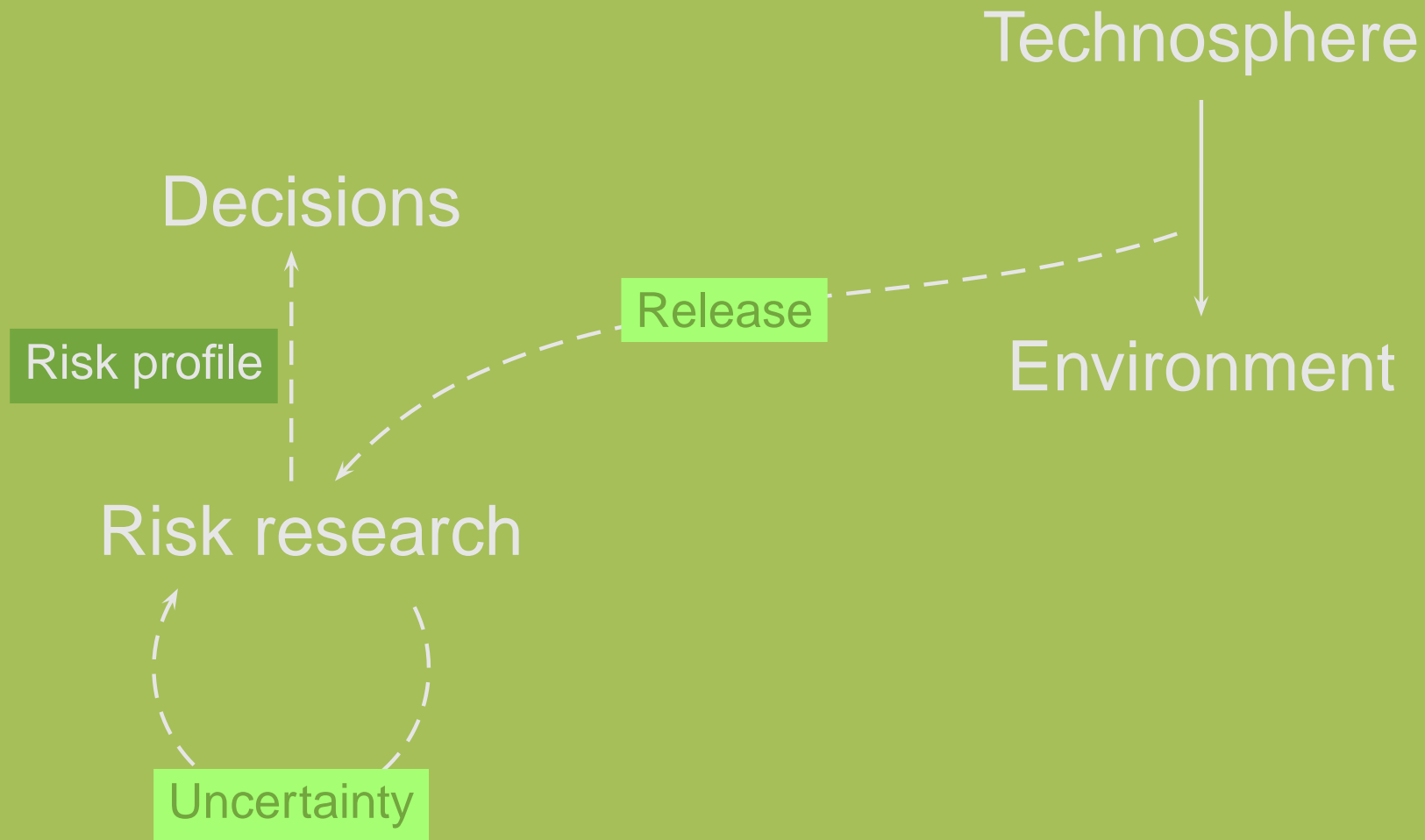




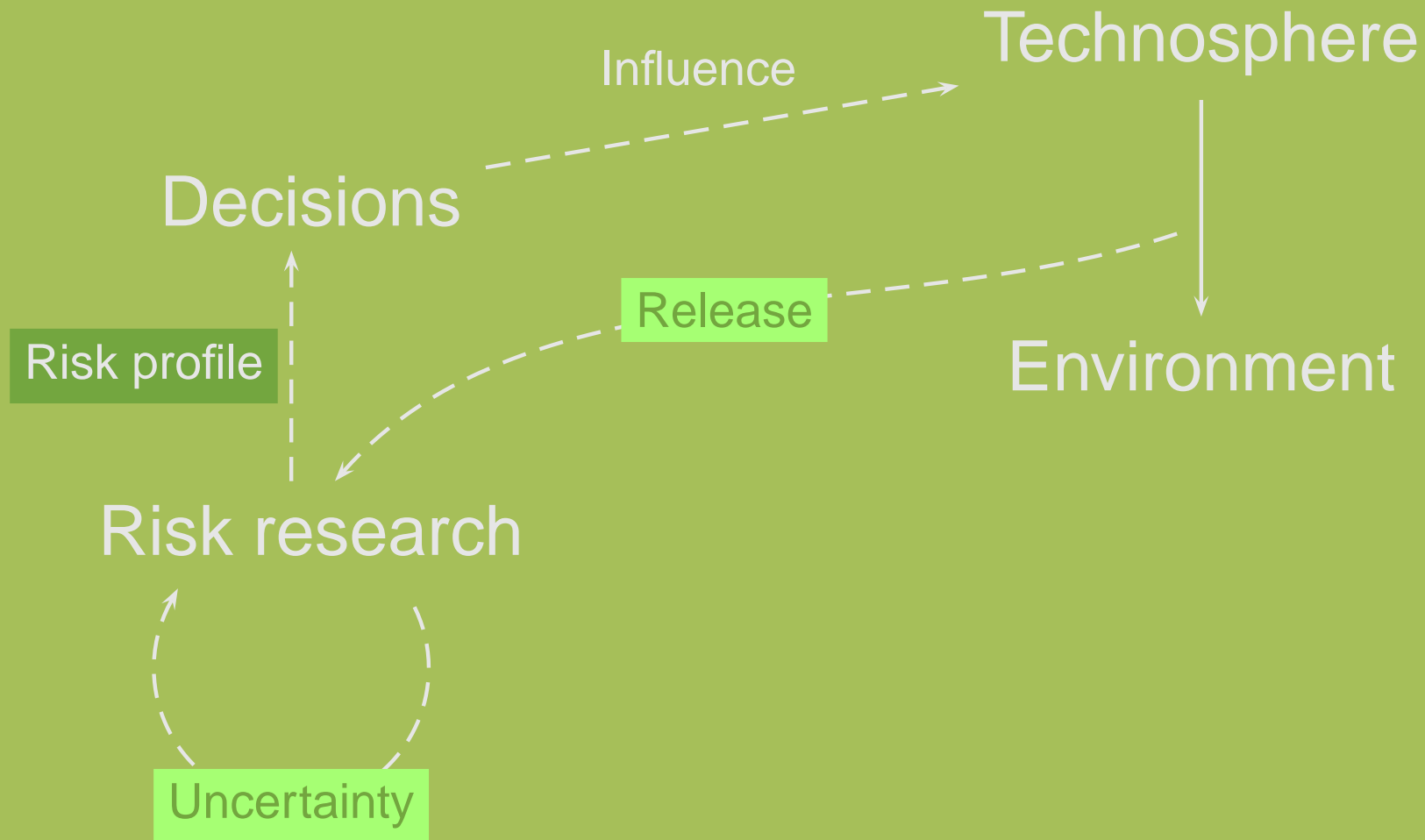
# Using five risk indicators



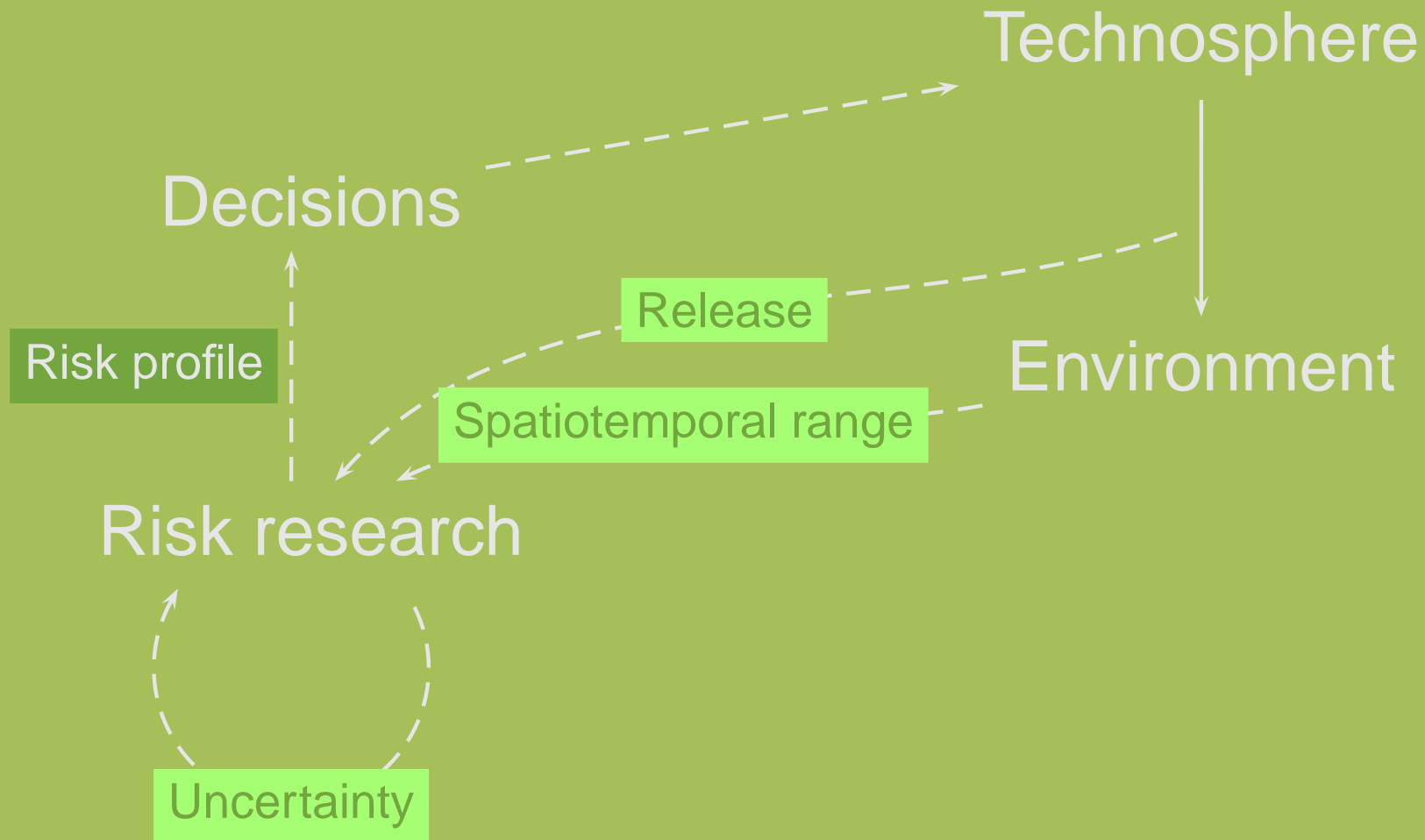
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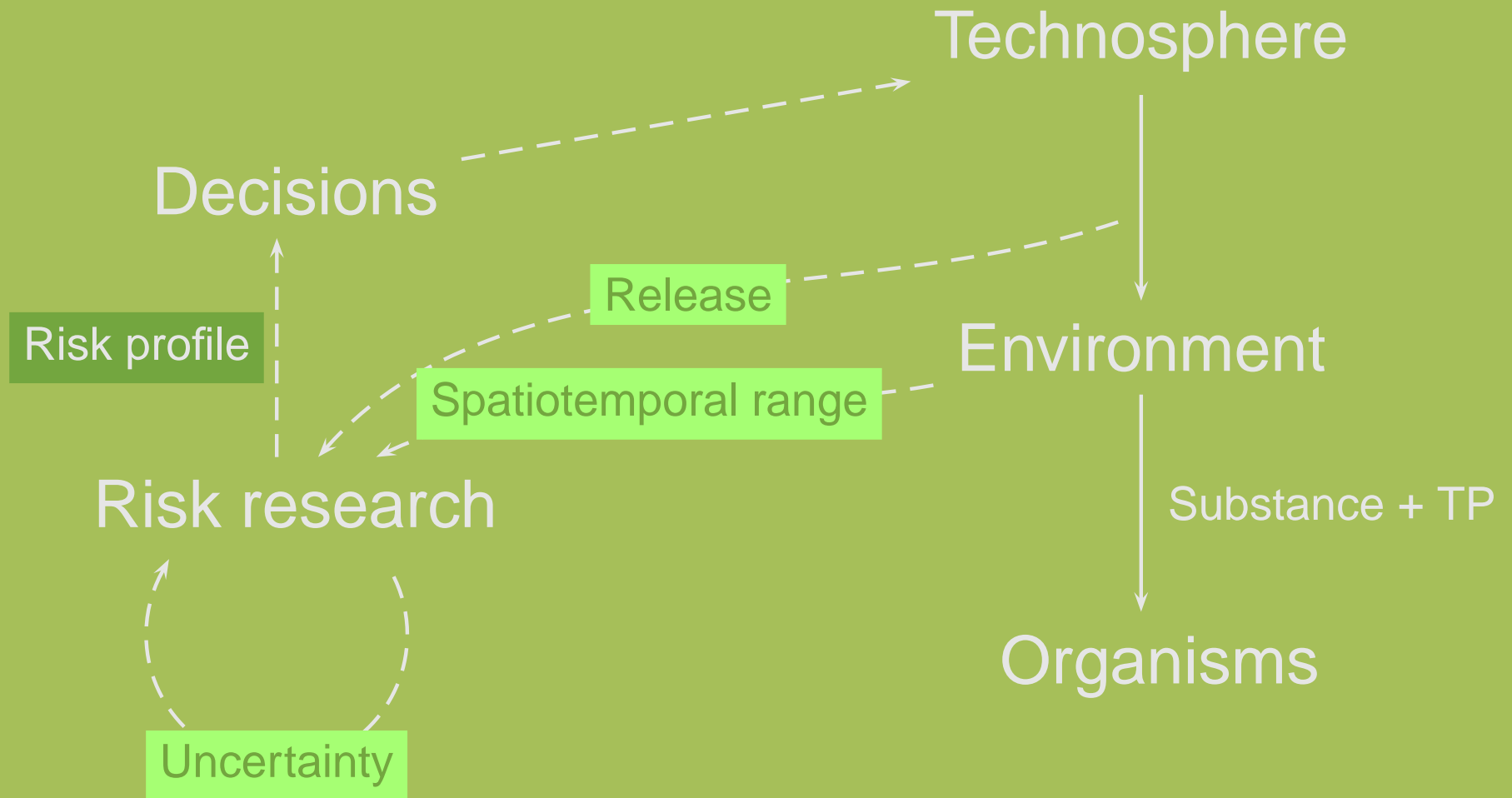
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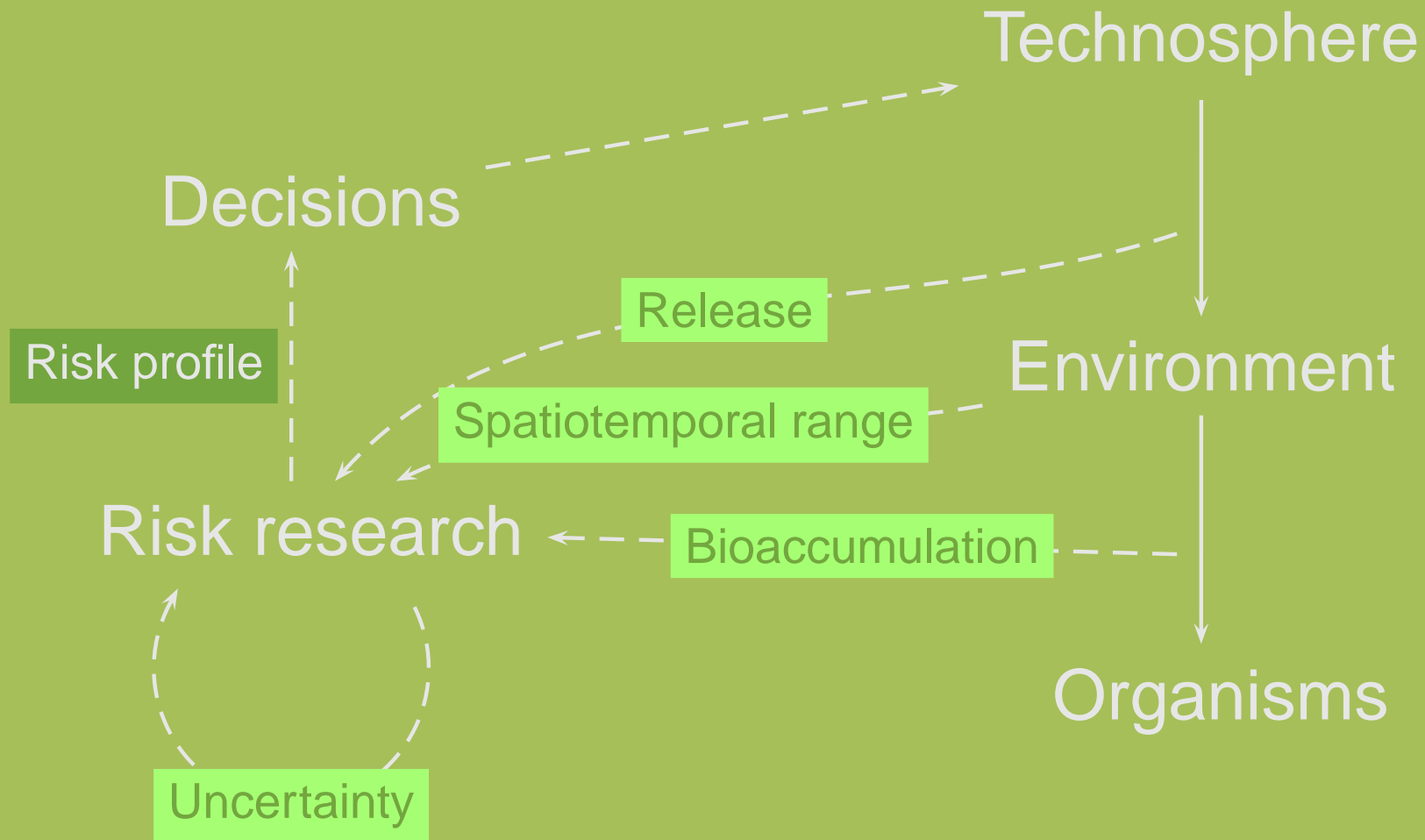
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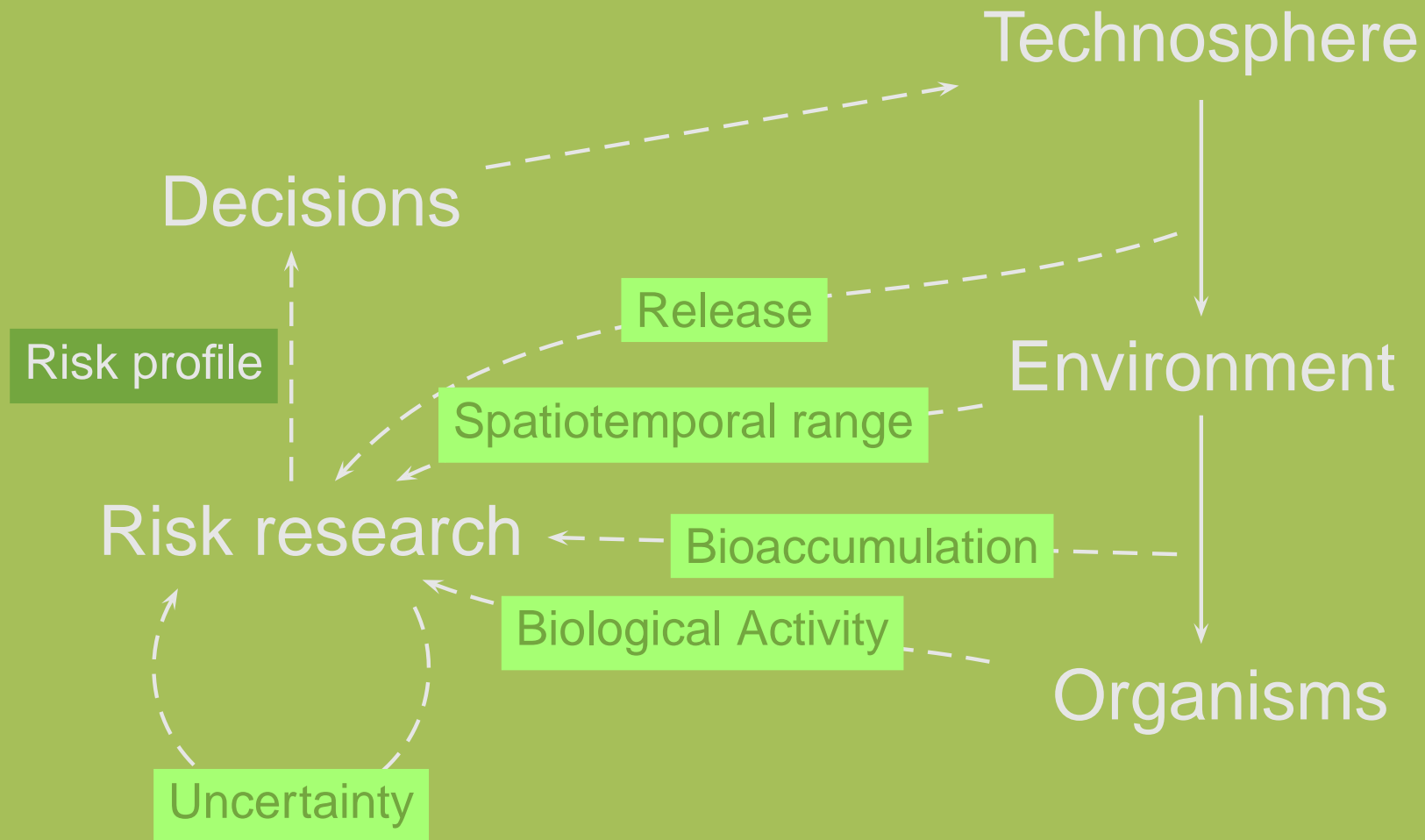
# Using five risk indicators



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# Input / into the environment

$$I = \sum_u f_u \cdot P_u$$

$I$  Input in tons per year

$u$  Index of use patterns

$P_u$  Production volume for use pattern  $u$

$f_u$  Fraction of  $P_u$  released to environment



# Release indicator R

$$R \propto \log_{10} I$$

$I$  Input in tons per year

# Spatiotemporal range indicator S

$$S \propto \log_{10} \frac{M_{\text{env}}}{I}$$

$M_{\text{env}}$  Mass in the environment at steady-state  
 $I$  Input in tons per year

# Spatiotemporal range indicator S

$$S \propto \log_{10} \frac{M_{\text{env}}}{I} = \log_{10} t_{\text{env}}$$

- $M_{\text{env}}$  Mass in the environment at steady-state
- $I$  Input in tons per year
- $t_{\text{env}}$  Residence time in the environment  
(Overall persistence)

# Assessment of S

- Define system boundaries

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- Calculate the fate parameter

# Mackay modelling levels

- I Equilibrium partitioning under steady state
- II As in I plus losses by advective transport and degradation
- III Nonequilibrium because of intermedia transport, steady state
- IV Same as III but unsteady state

e.g.: Mackay D et al. (1996) *Environ Toxicol Chem* 15:1618-1626



# Spatial setups

- Local model
- Regional model
- Global model
- Nested model

# Examples

- Mackay I: regional, Level I

# Examples

- Mackay I: regional, Level I
- EUSES: nested, Level III

# Examples

- Mackay I: regional, Level I
- EUSES: nested, Level III
- Scheringers ring model: global, Level III

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- Wantias model: global, Level IV

# Examples

- Mackay I: regional, Level I
- EUSES: nested, Level III
- Scheringers ring model: global, Level III
- My antifouling model: global, Level III
- Wantias model: global, Level IV
- Scheringers chain model: global, Level IV

# Conclusions

## Fate models

- provide insight



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