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ConsExpo

Consumer Exposure Modeling

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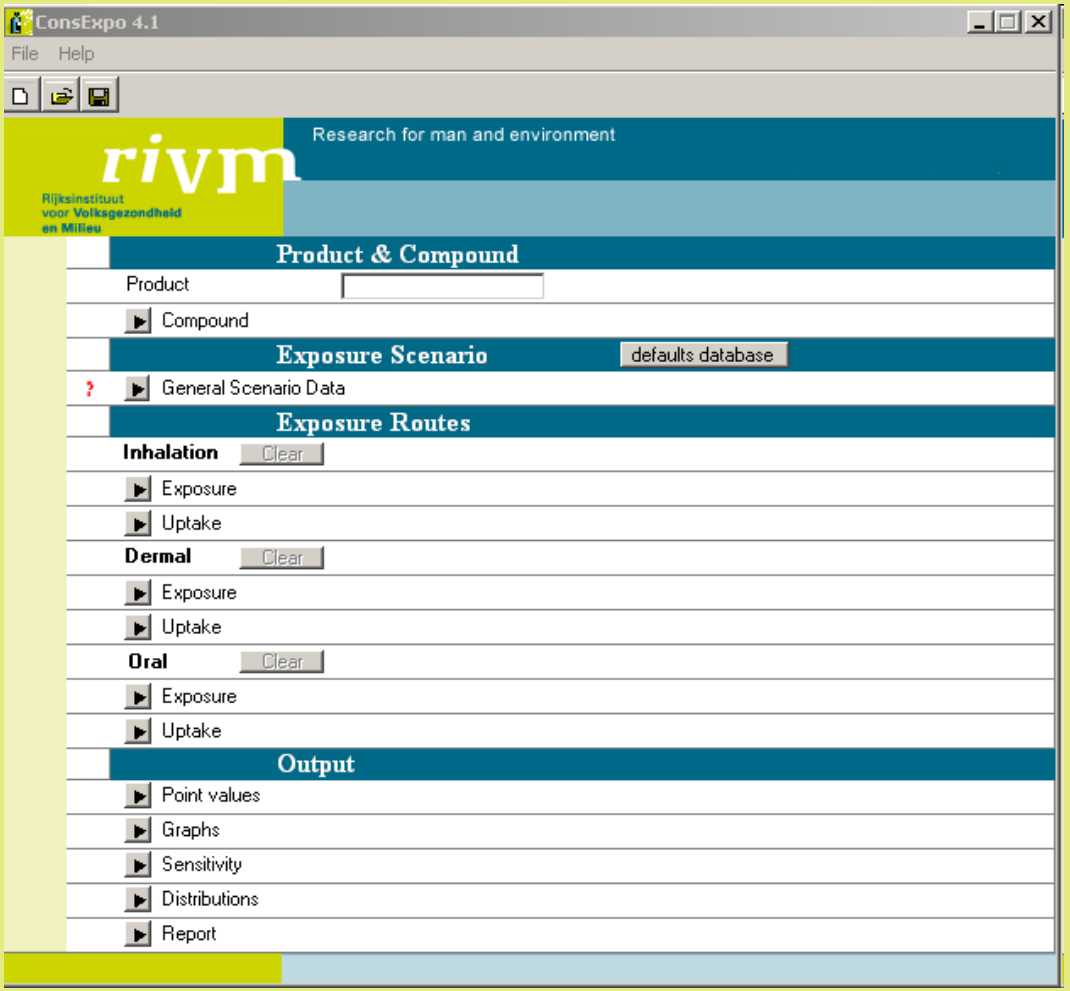
Consumer Exposure Modeling Tool

Dutch Food and Consumer Product Safety Authority



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Modelling consumer exposure to chemicals in consumer products: ConsExpo

Set of models describing various exposure processes

- Multi-route
  - inhalation
  - dermal
  - oral
- Multi-tiered
  - first order screening models
  - more detailed models
  - population exposure calculation tools (limited)

Models in ConsExpo

Inhalation:

- Vapours
- Aerosols

Dermal:

- Direct dermal contact
- Rubbing of surface
- Migration from material direct in contact with the skin
- Diffusion through product, then direct in contact with skin

Oral:

- Ingestion
- Mouthing
- Migration from food contact (packaging) materials

ConsExpo work flow

Compound
-vapour pressure
-molecular weight
-Kow
- absorption fraction

Product
-composition
-migration rate
-diffusion coefficient
-aerosol size distribution

single event exposure simulation

inhalation	dermal	oral
vapours	transfer of residu from surface	accidental swallowing
aerosol spray	migration from product	leaching from product
	diffusion from product	migration from packaging material

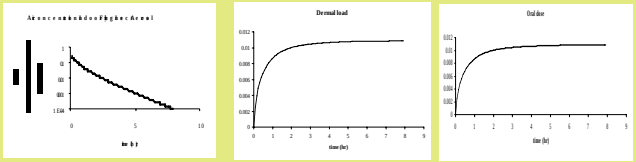
exposed person
-amount used
-exposure duration
- inhalation rate

Residence
-room size
- ventilation

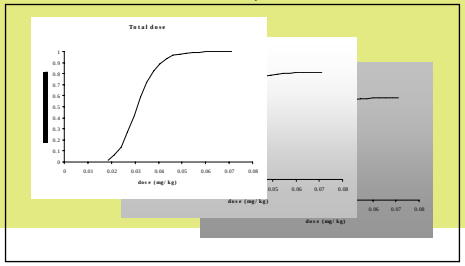
single event exposures

- **air concentration**
- **inhaled event dose**
- **dermal load**
- **dermal event dose**
- **oral event intake**
- **total event dose**

air concentration | **dermal load** | **acute oral intake**



exposure pattern
- exposure frequency



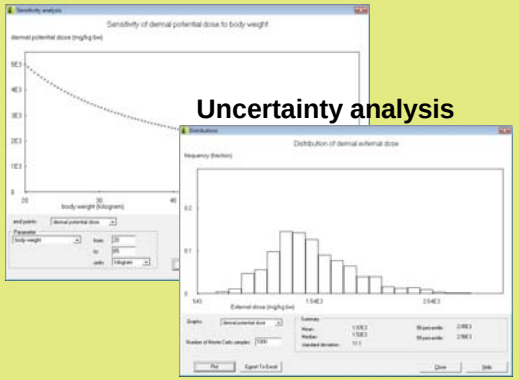
chronic exposures

- **-inhaled dose**
- **-dermal dose**
- **-oral dose**
- **-total dose**

Analysis

Sensitivity analysis

Uncertainty analysis



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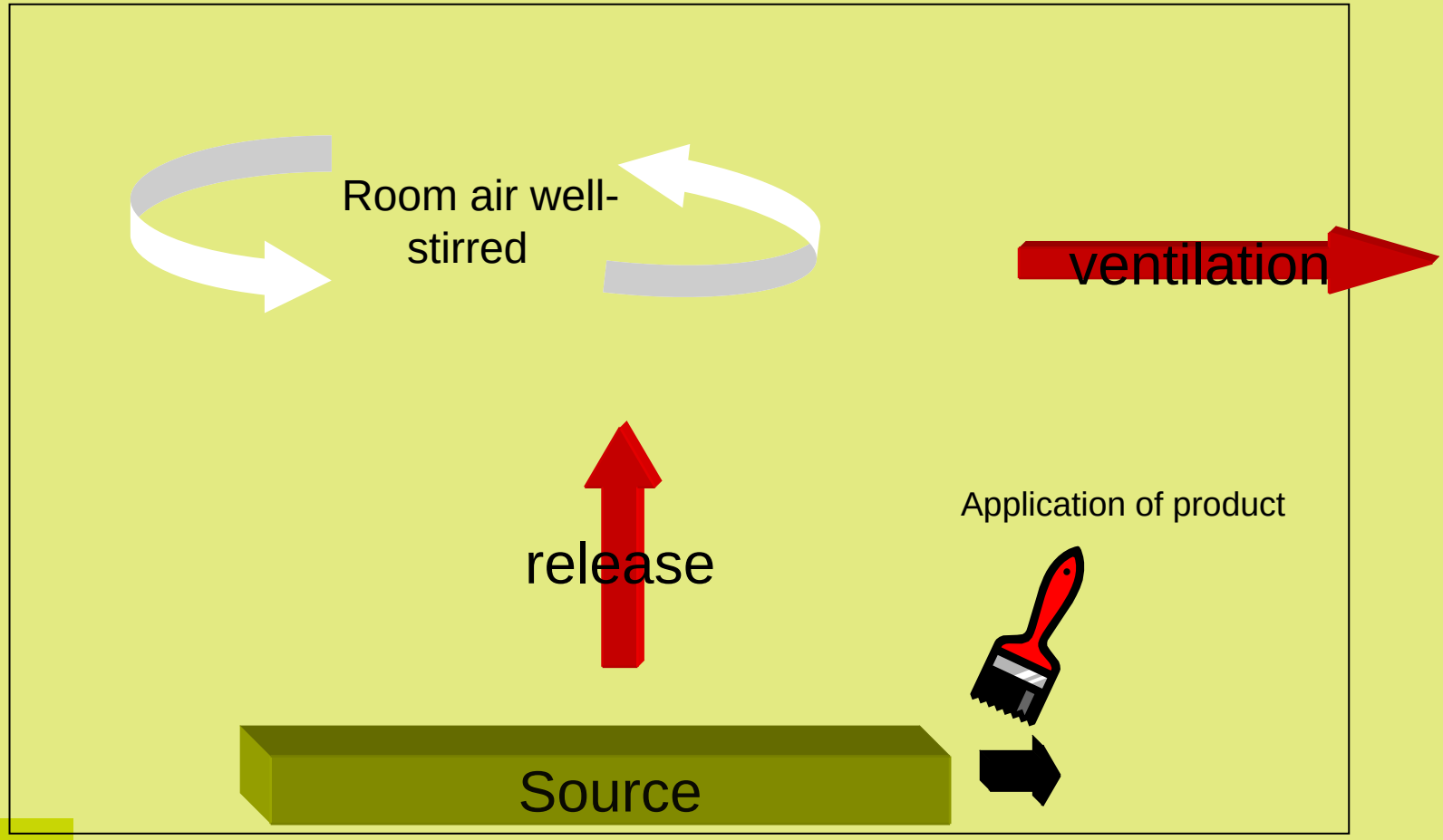
Inhalation models: vapours



Inhalation models: vapours

Release modes

- Instantaneous: screening of upper limits of air concentration (RIP inhalation a)
- Constant rate: release at a constant rate during a fixed time (use if a reasonable estimate can be made of release duration)
- Evaporation: model explicitly estimates the release of chemical due to evaporation

Inhalation models: vapours

Evaporation

- Evaporation of chemical from surface, driven by difference in pressure and saturated vapour pressure
- Evaporation surface:
  - Constant (i.e. previously treated surface)
  - Increases in time (i.e. as in painting/cleaning/treating a surface)
- Matrix of product (ideal liquids)
  - Pure substance
  - Mixture (Raoult's law)

c1

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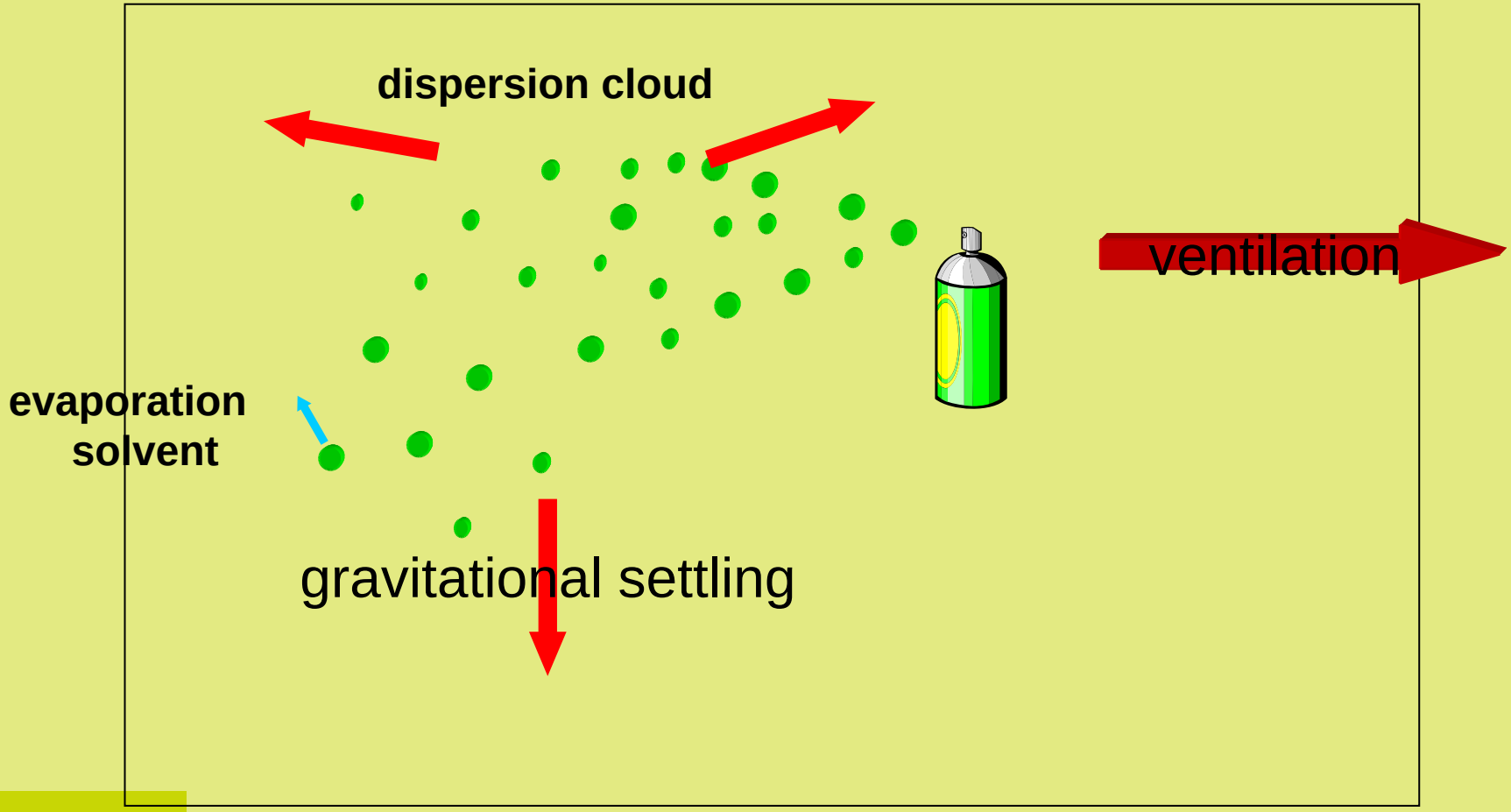
c1 valid only approximately for liquids, extrapolation uncertainty

christiaan; 02/05/2005

Inhalation models: sprays, air concentrations



Inhalation of aerosols: dosimetry and particle size

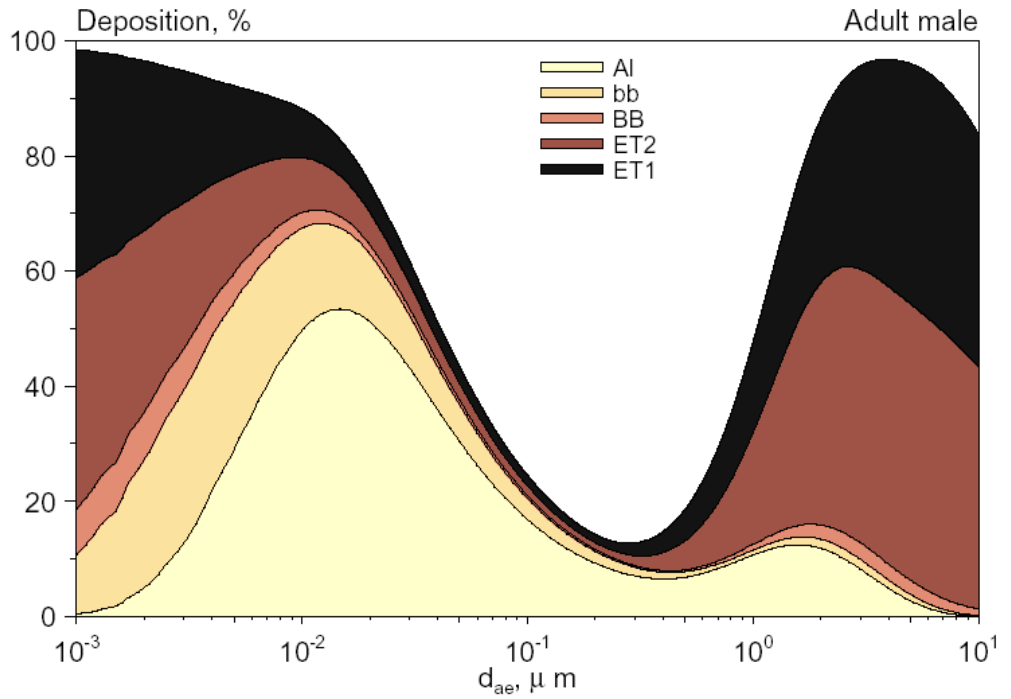


Figure 7. Deposition of aerosols in the lung tract (Freijer et al., 1997). The fraction that is not deposited in the extrathoracical airways, ET1 and ET2 in the figure, is considered to be the respirable fraction. Al-alveoli, bb=bronchioles, BB=bronchia, ET1=extrathoracical region 1, ET2=extrathoracical region 2.

Inhalation models: sprays

Non (low)-volatile substances released as an aerosol spray

Simplifying assumptions

- Instantaneous mixing of indoor air
- Removal of aerosol by gravitational sedimentation and ventilation only (aerosol diameters ≥ 0.5 μm)
- Immediate evaporation of solvents
- Deposition in respiratory tract:
  - diameter < inhalation cut-off: inhalation exposure
  - diameter > inhalation cut-off: oral exposure

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c3 valid only approximately for liquids, extrapolation uncertainty

christiaan; 02/05/2005

Distributional (probabilistic) calculations

Account for:

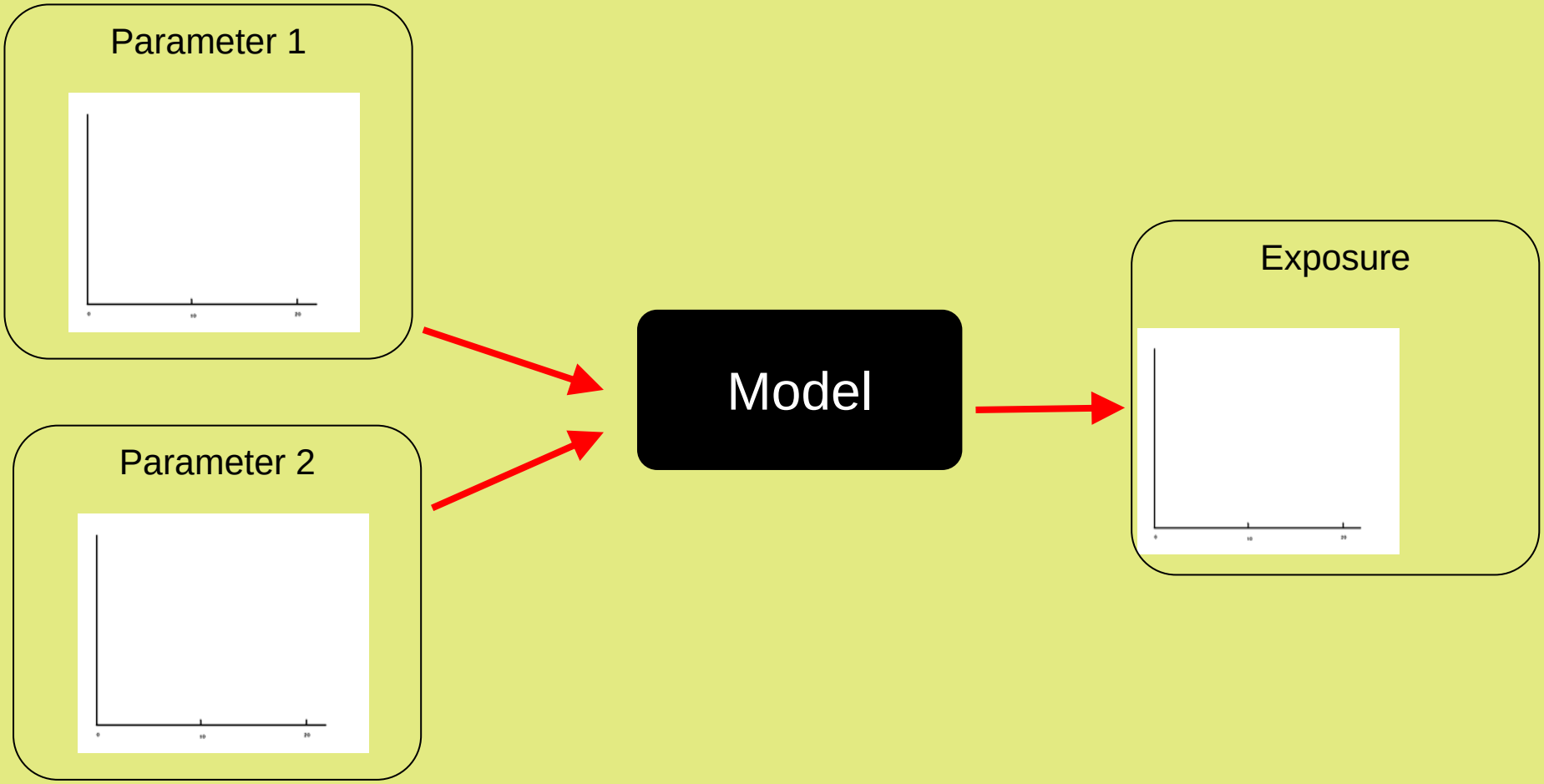
- Uncertainty (variation due to imperfect/incomplete knowledge)
- Variability (natural variation of parameter)

Tool: Monte Carlo analysis

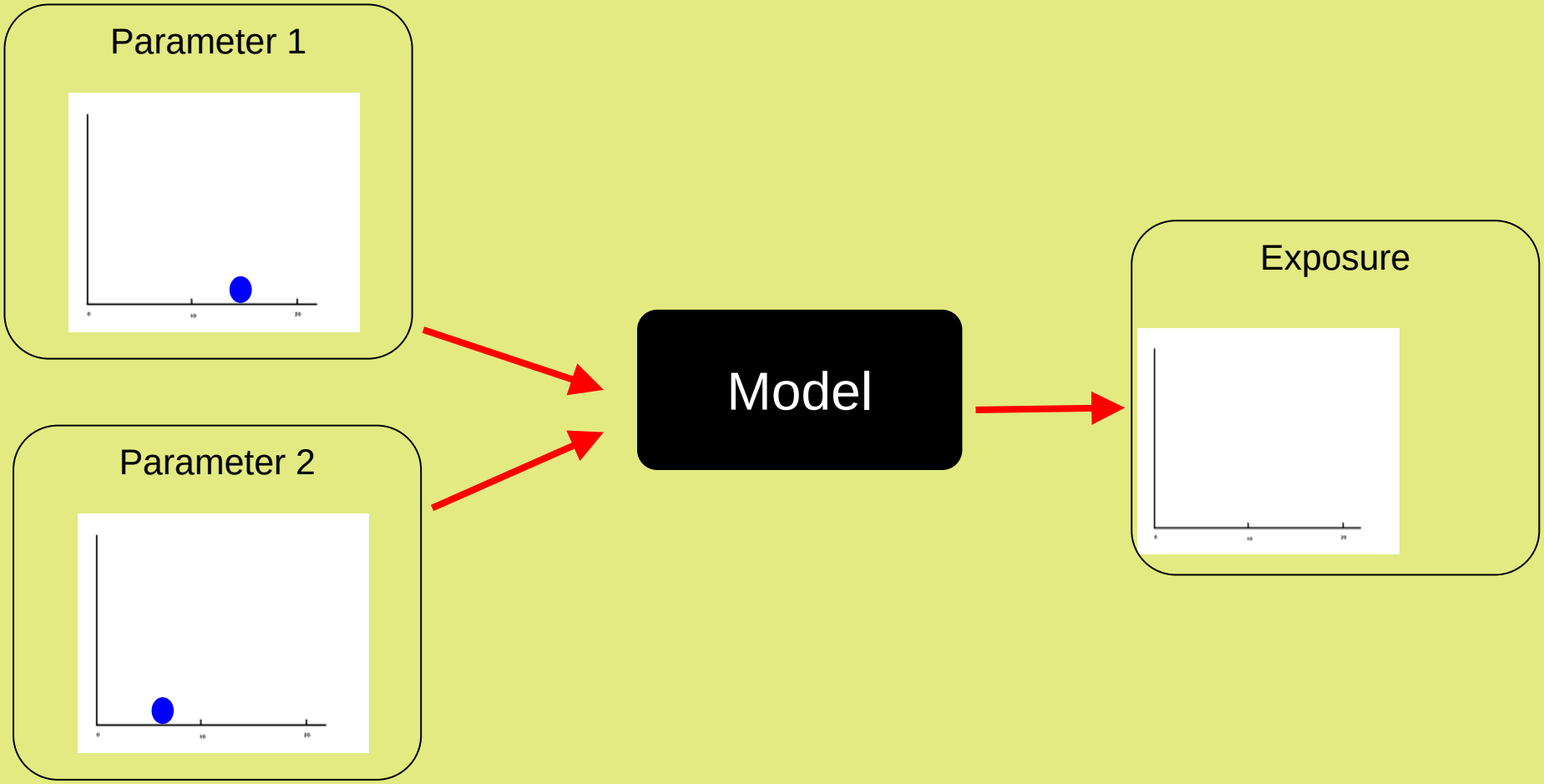
Limitations ConsExpo:

- Only 1-dimensional Monte Carlo analysis (no distinction can be made between uncertainty and variability)
- No correlations are taken into account

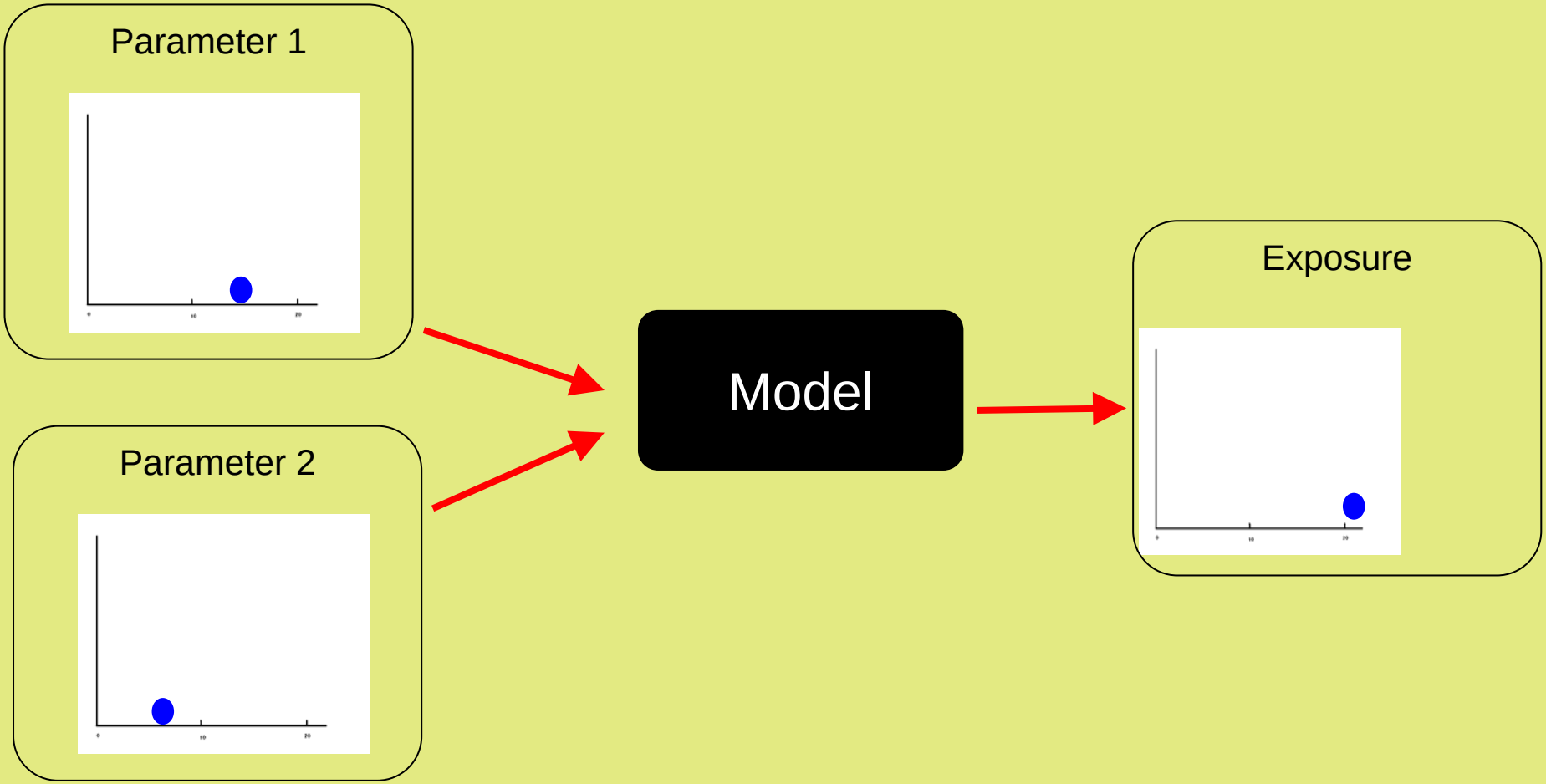
Distributional (probabilistic) calculations



Distributional (probabilistic) calculations

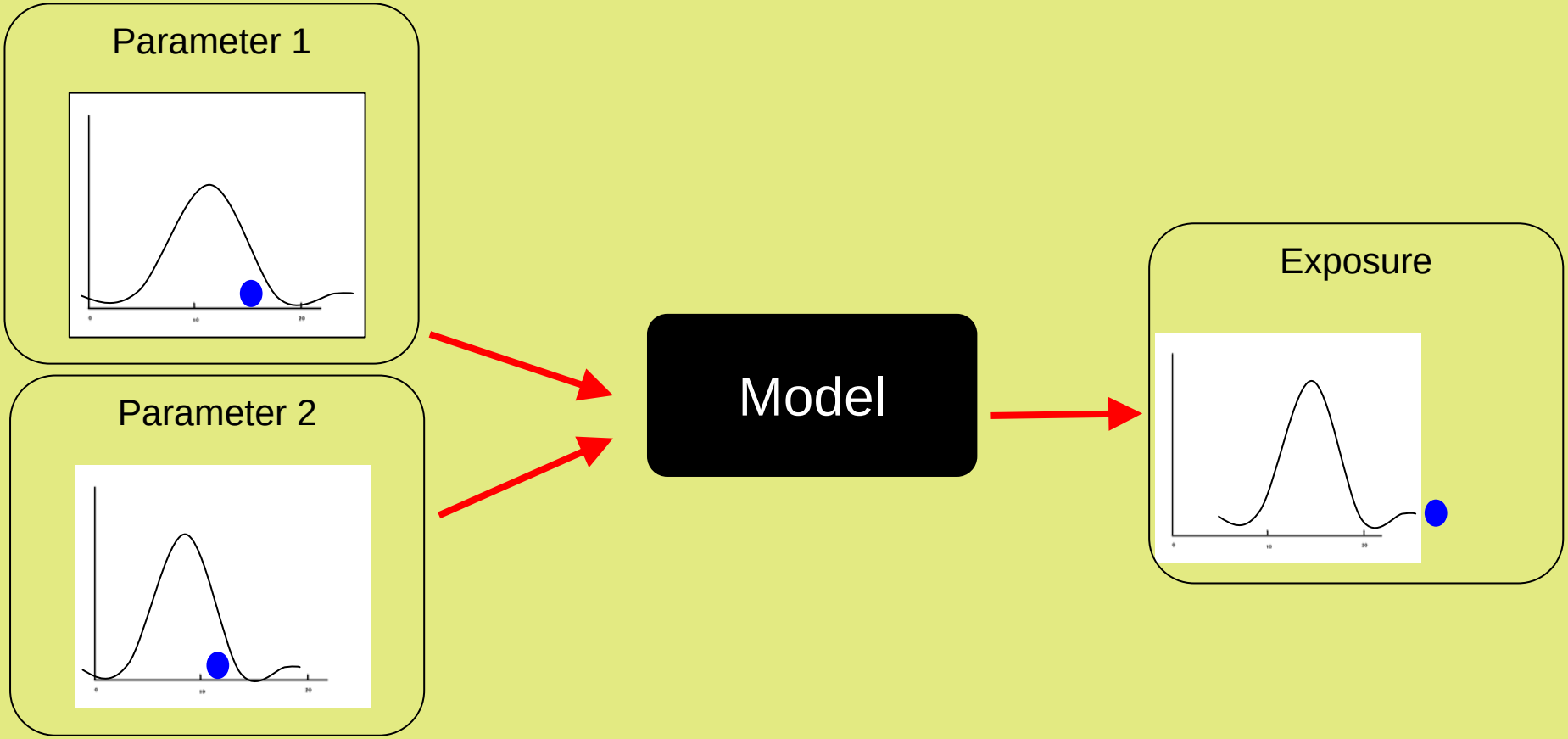


Distributional (probabilistic) calculations



Distributional (probabilistic) calculations: high exposed person estimate

c2



'conservative' point estimates for parameter inputs:
unknown degree of over-estimation exposure

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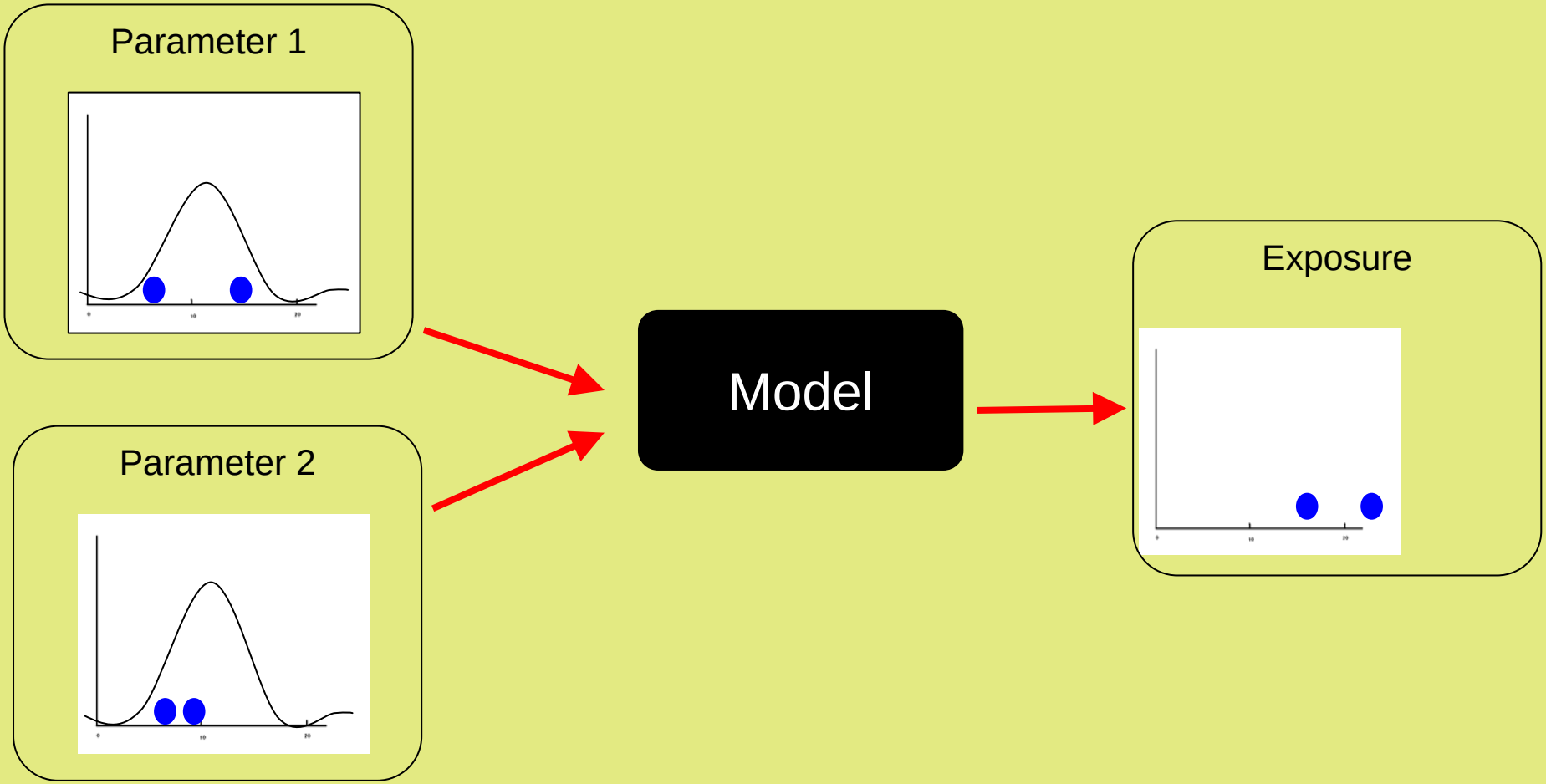
c2 single, high exposed person estimate

christiaan; 02/05/2005

Distributional (probabilistic) calculations



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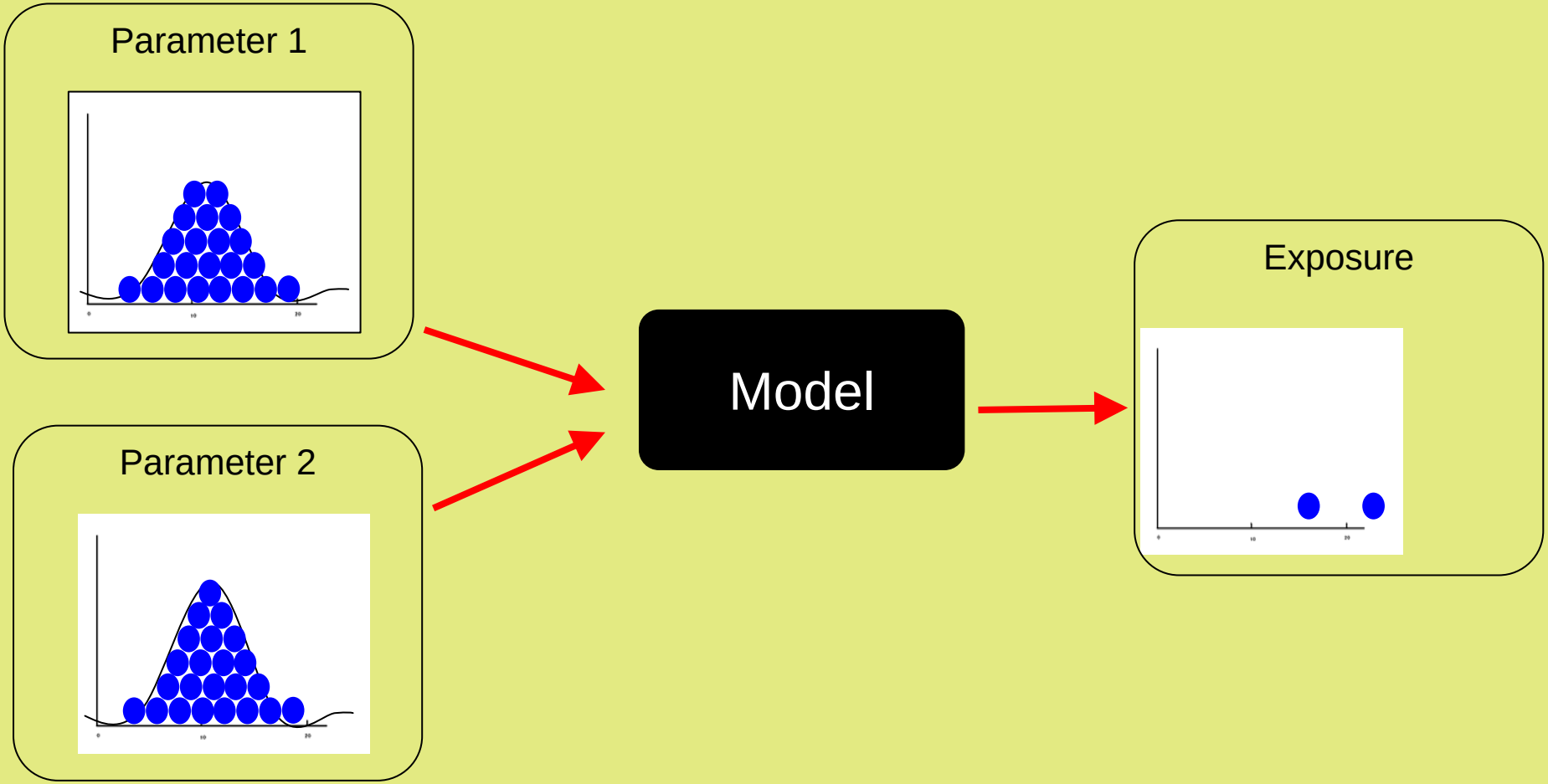

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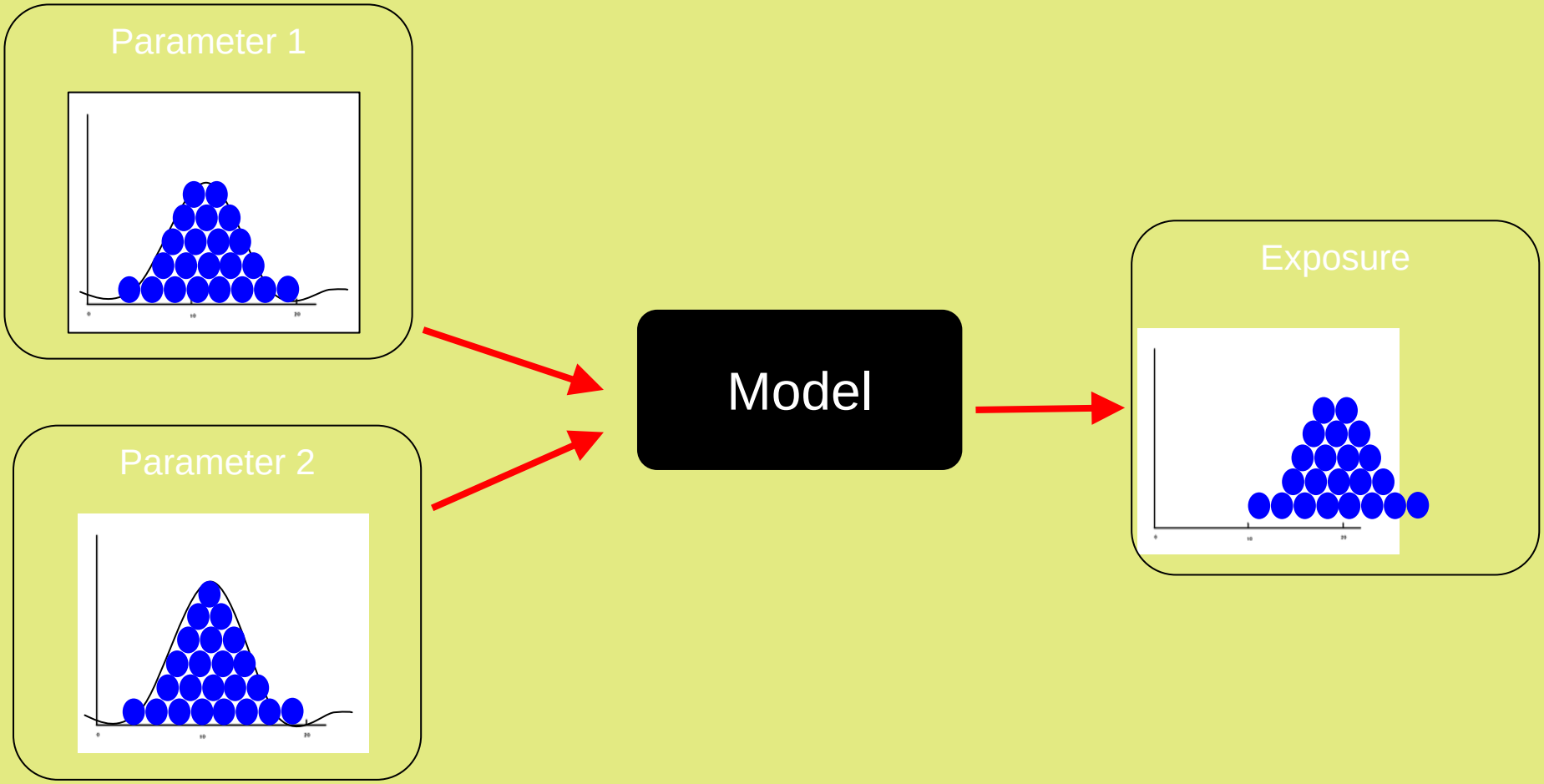


Distributions

Uniform

- Upper bound
- Lower bound

Triangular

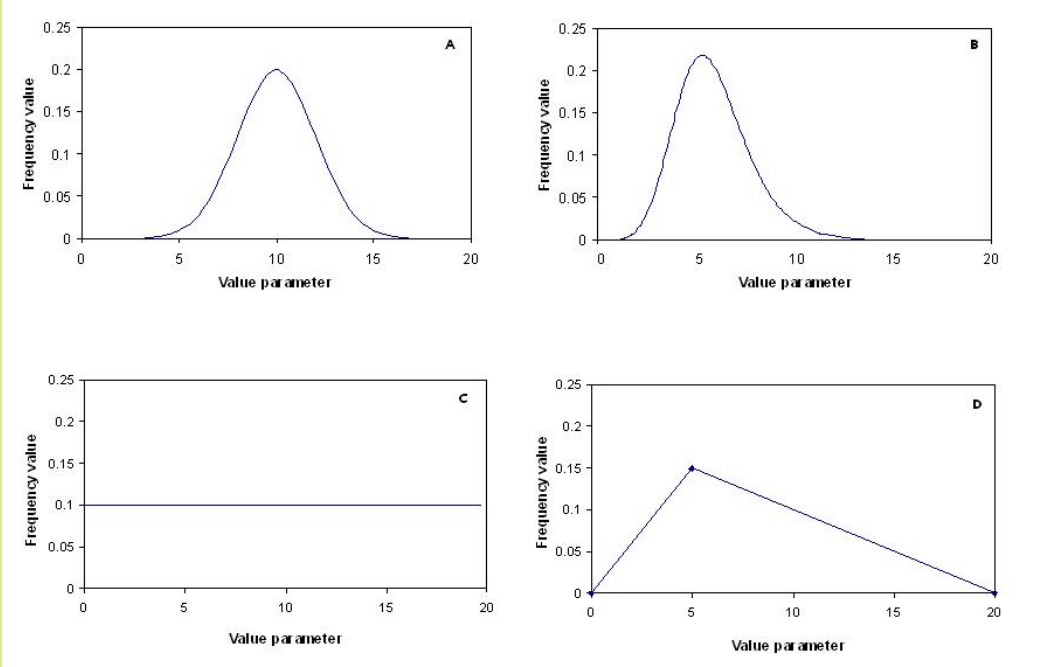
- Location (minimum)
- Scale (maximum)
- Shape (max. probability)

Normal

- Standard deviation
- Mean

Lognormal

- Median
- Coefficient of Variation (S.d./Mean)



Sensitivity analysis

Dependence of model outcome on variations of input parameters

ConsExpo: 1-dimensional sensitivity analysis: variation of 1 parameter, other parameters are fixed.

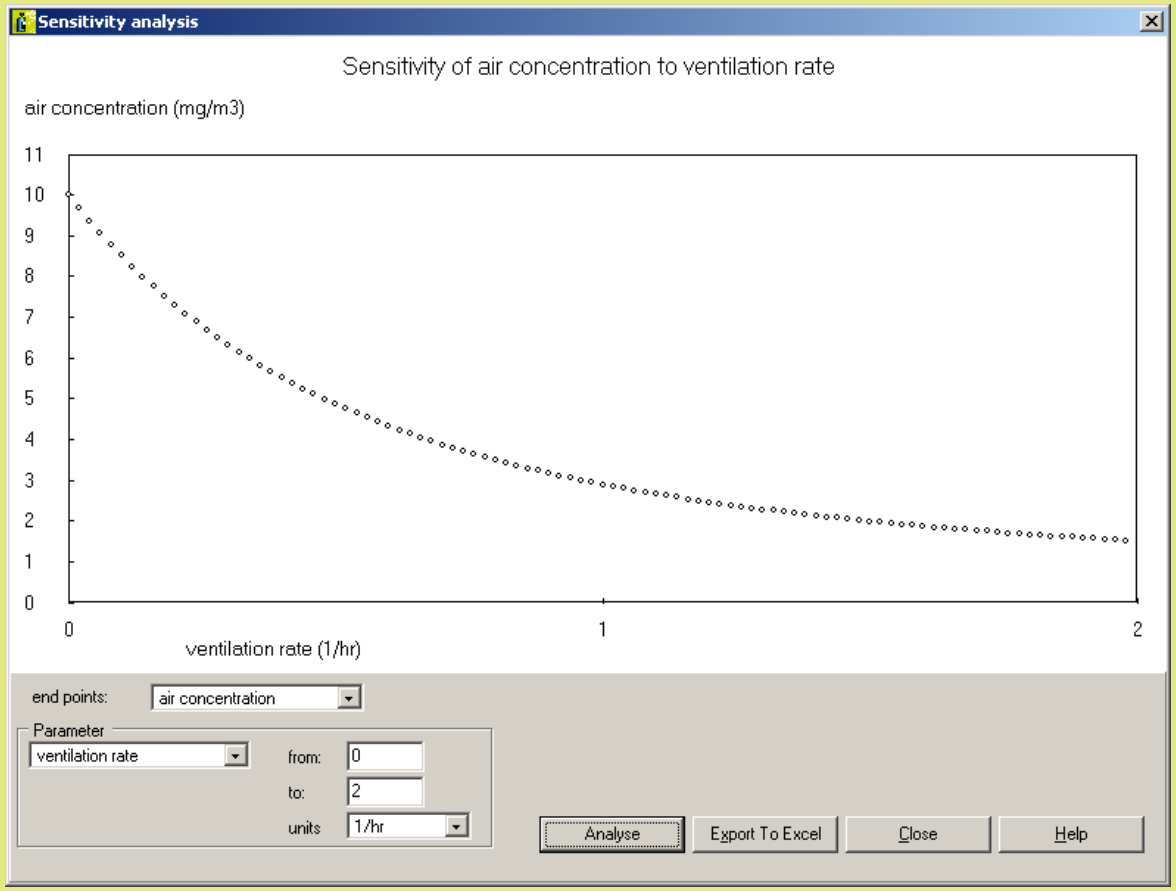
Sensitivity model depends on:

- Model structure
- Range and value parameter
- Values of other parameters

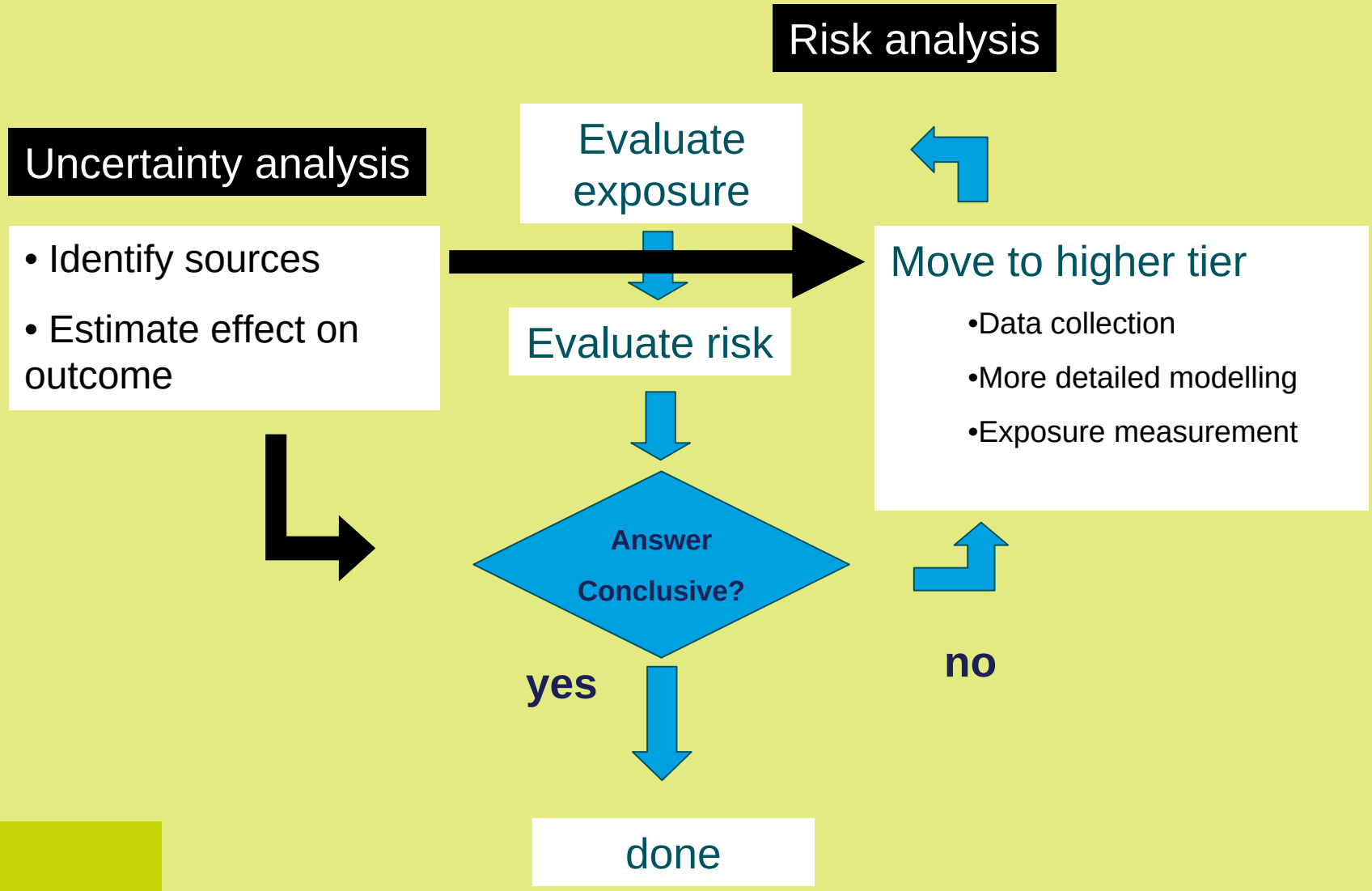
Study importance of parameter

Sensitivity analysis

- Effect of ventilation on air concentration in inhalation exposure
- range of ventilation rate: 0-2 airchanges/hr



Putting it together: tiered risk analysis



Sources of Uncertainty

- Scenario uncertainty
  - wrong or incomplete information
  - not identifying important route/pathway
  - …
- Model uncertainty
  - extrapolation uncertainty
  - modeling errors
  - over-simplification
  - ….
- Parameter uncertainty
  - measurement errors
  - data derived from a small sample
  - extrapolation uncertainties
  - …..

Parameter Uncertainty Analysis

- Evaluate quality of data set
  - Qualitative: good/poor
  - Estimate ranges (minimum and maximum values)
  - Derive uncertainty distributions
- Evaluate sensitivity of assessment to parameter
  - Interval estimate: evaluate exposure for high, medium and low values of parameter
  - 1-dimensional sensitivity: vary parameter continuously over entire range
  - Probabilistic (1-dimensional): Monte Carlo simulation with probability distribution of the parameter
- Evaluate uncertainty of all parameters combined
  - Factorial design: combine evaluations of high, medium and low for all parameters
  - Probabilistic: use distributions of all parameters to perform Mont Carlo analysis

Developments

- Model validation
- Emissions of substances from solid matrices
- Multiple product exposures
- Enhanced probabilistic capabilities (correlations, presentation)
- Version 5 (beta 2008)

ConsExpo

ConsExpo and fact sheets available at:

www.consexpo.nl

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