Uncertainty and variability in the exposure reconstruction of chemical incidents

The case of acrylonitrile

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NVvA symposium 2015

2015-03-19

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CHEMICAL SUBSTANCES RISK ASSESSMENT

Chemical incidents

DMMP & Isopropanol

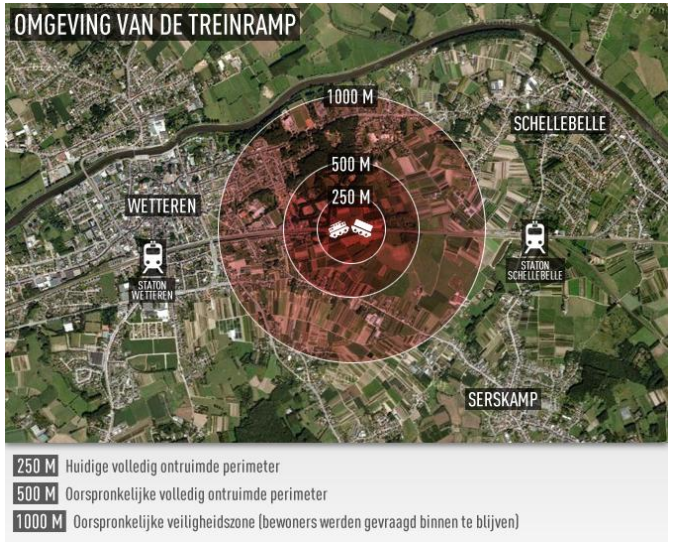
El Al Boeing, Amsterdam

Oct 4, 1992

Acrylonitrile

Train disaster, Wetteren

May 4, 2013



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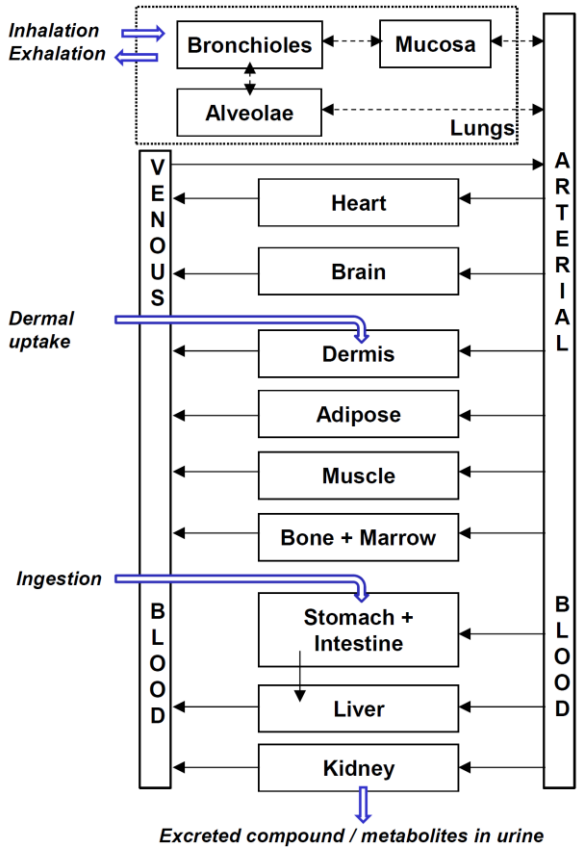
Exposure assessment possibilities



External Exposure (Measure / Model)

Internal Exposure (Measure / PBTK Model)

"Reverse Dosimetry"

Questions & Aim

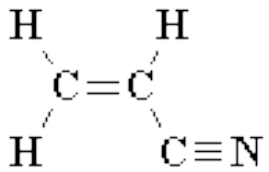
- What is the exposure during a chemical incident?
  - Air measurement data are scarce (or lacking)
  - Often only blood samples available (days or weeks after incident)
  - Exposure duration?
  - Exposure dynamics?
  - Different exposed groups (rescue workers, residents)

- **Aim**:

  Characterization of uncertainty and variability in the exposure reconstruction of chemical incidents

Case study acrylonitrile

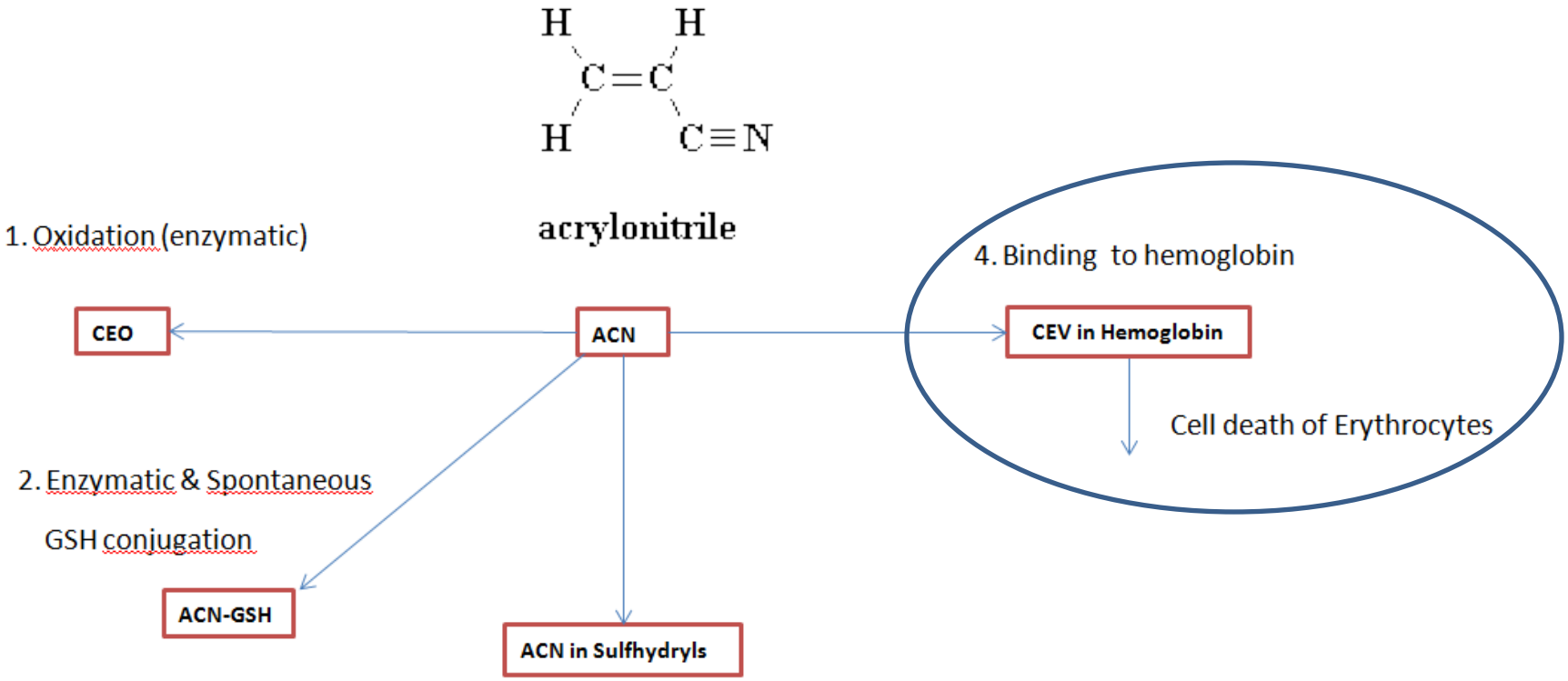
- Chemical incident (*Bader et al. 2006*)
  - Decontamination of tank wagons containing acrylonitrile
  - Cleaning workers (n=4, 1 entering tank wagon)



acrylonitrile

Case study acrylonitrile (2)

- Sample collection (*Bader et al. 2006*)
  - Blood samples after 25 days and 85 days
  - N-2-cyanoethylvaline (CEV) in hemoglobin



Method

Reversed dosimetry

Principle of Exposure Conversion Factor (ECF) *(Liao et al. 2007)*

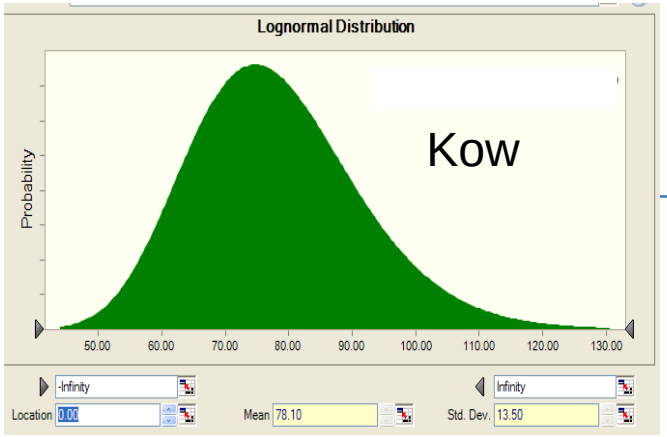
Forward Dosimetry

$$ECF = \frac{C_{bl,\ t\text{-}m}}{C_{air,\ t\text{-}exp}} = \text{constant}$$

$$\frac{C_{bl,\ t\text{-}m}}{ECF} = C_{air,\ t\text{-}exp}$$

Method

Sources of variability and uncertainty

X → 

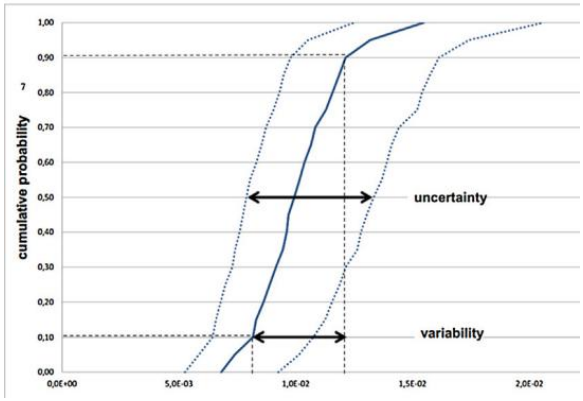
→ Y ± …% ?

(interindividual) Variability

- Human physiology

Uncertainty

- Exposure duration
- Phys-Chem properties



Method

Nested Monte Carlo Simulation

- 2 scenarios with fixed air concentrations:
  - 3 ppm ACN in air for 5 minutes
  - 3 ppm ACN in air for 60 minutes

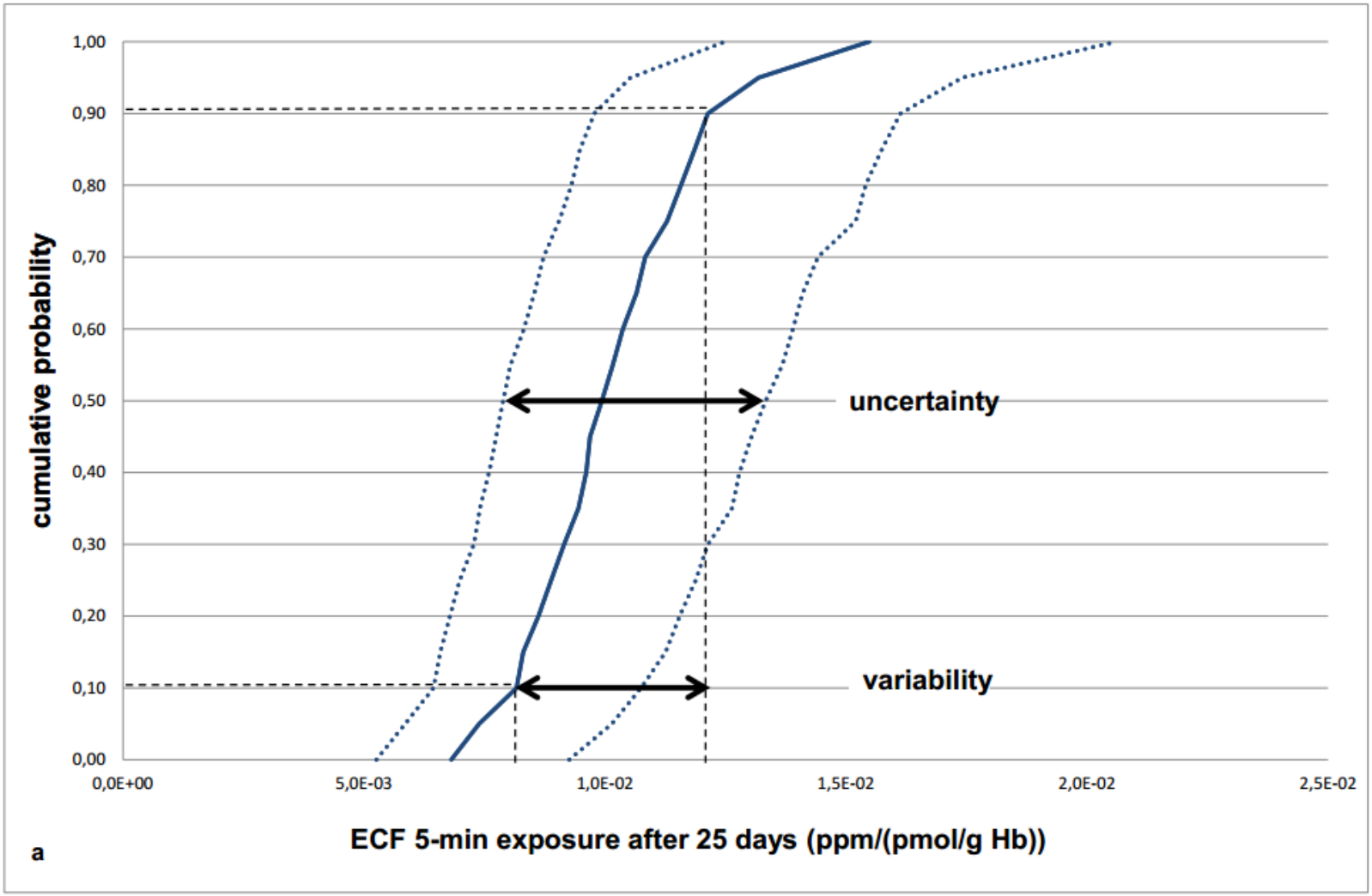
- Calculation of ECF-distribution per scenario

  (based on 10.000 model simulations)

- Calculation of air concentration during incident based on individual blood samples (CEV) and ECF distribution for each worker

Results

ECF probability plot



Results

Reconstructed air concentrations

Recalculated air concentrations ACN at the time of the incident.

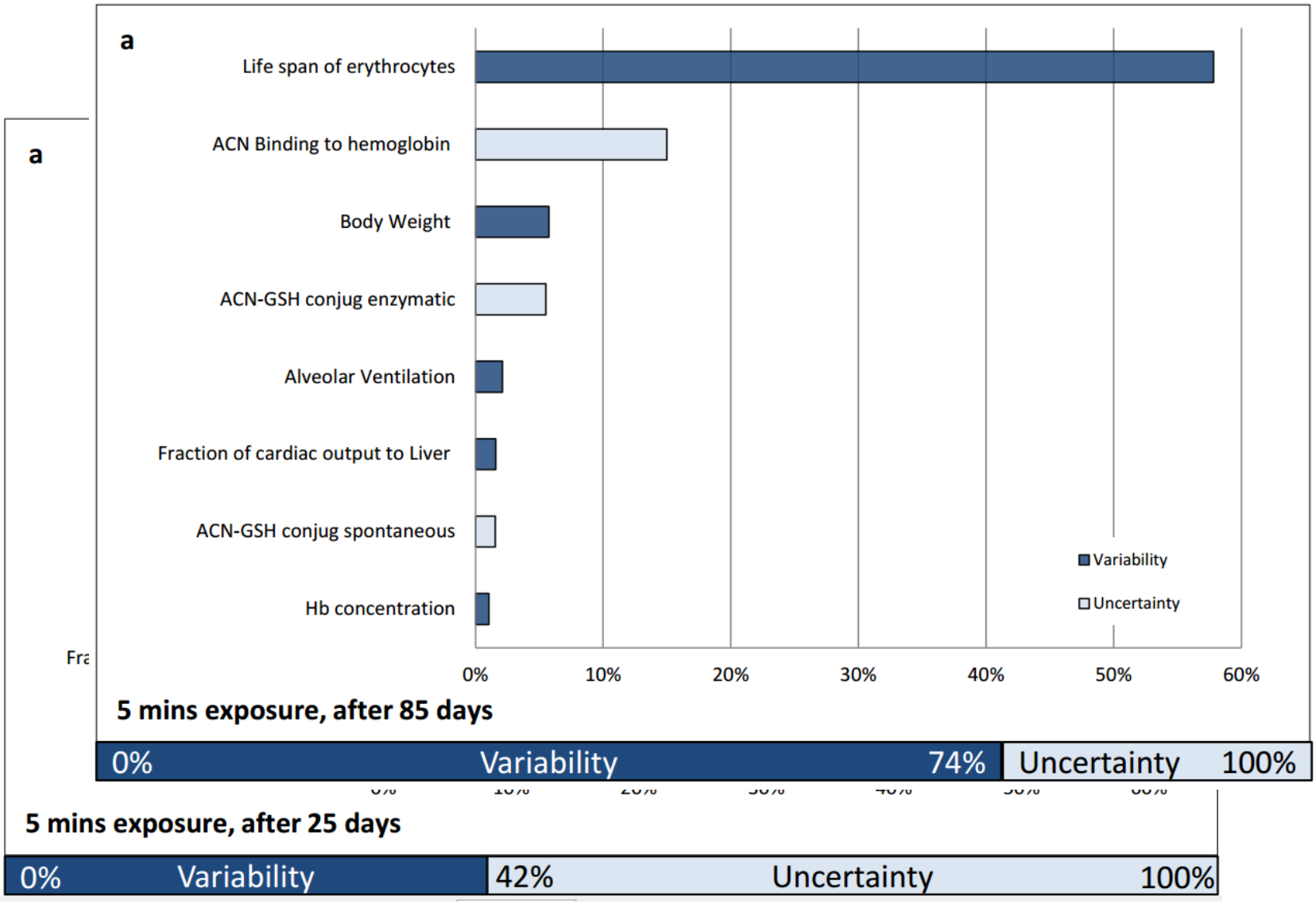
Exposure scenario			85 days after the incident	
No.	Exposure duration	Worker	Measured concentration CEV (pmol/g Hb)	Reconstructed air concentration ACN at the time of the incident (ppm)
1.	5 min	1	995	37.9 (18.2–112.9)
		2	88	3.3 (1.6–10.0)
		3	406	15.5 (7.4–46.1)
		4	283	10.8 (5.2–32.1)
2.	60 min	1	995	2.7 (1.5–5.6)
		2	88	0.2 (0.1–0.5)
		3	406	1.1 (0.6–2.3)
		4	283	0.8 (0.4–1.6)

- Median reconstructed air concentrations ranged from 0.5 – 38 ppm (depending on scenario)
- Acute limit values of 25 ppm (NL, RIVM) and 57 ppm (US, EPA)

-> for 1 worker the predicted p-90 value > EPA limit value (5-min scen. 85 days)

Results

Parameter importance



Conclusions and implications

- Conclusions
  - Method seems suitable for exposure reconstruction
  - Predicted ranges within a factor 3 with this method
  - Uncertainty in exposure duration most significant source

- Recommendations
  - Strict documentation of ‘exposure scenario’ after incident
  - Collect urine/blood samples a.s.a.p. to decrease uncertainty
  - Collect human physiological data from victims to decrease variation in modeled results (up to 20% in this case)

Thank you for your attention

Questions?
Suggestions?
Remarks?

Toxicology Letters 231 (2014) 337–343

Contents lists available at ScienceDirect

Toxicology Letters

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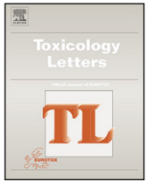

Uncertainty and variability in the exposure reconstruction of chemical incidents – the case of acrylonitrile

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HIGHLIGHTS

- Exposure to acrylonitrile during a chemical incident was reconstructed.

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