Stoffenmanager

Working safely with hazardous substances

Calibration and validation

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BECO
RETURN ON SUSTAINABILITY

- Stoffenmanager inhalation model
- Calibration and cross-validation
- Summary and discussion

Stoffenmanager inhalation model

- Freely accessible web-based tool (Dutch, English, (German))
  - (https://www.stoffenmanager.nl)

- Initially a prioritisation tool
  - Based on the source-receptor model (Cherrie e.a. Occup.Hyg 1996;3:75-83)
  - Marquart *et al. Ann.Occup.Hyg.* 2008;**52**(6):429-441

Example: Bagging product

NF and/or FF exposure		NF
Background	A	0.03
Intrinsic emission	E	0.3
Handling	H	10
Localized controls	LC	0.3
General ventilation	GV	0.1
Separation	Imm	1

$$Score = \{[background\ ] + [NF\ \_emission\ ] + [FF\ \_emission\ ]\} * immission$$

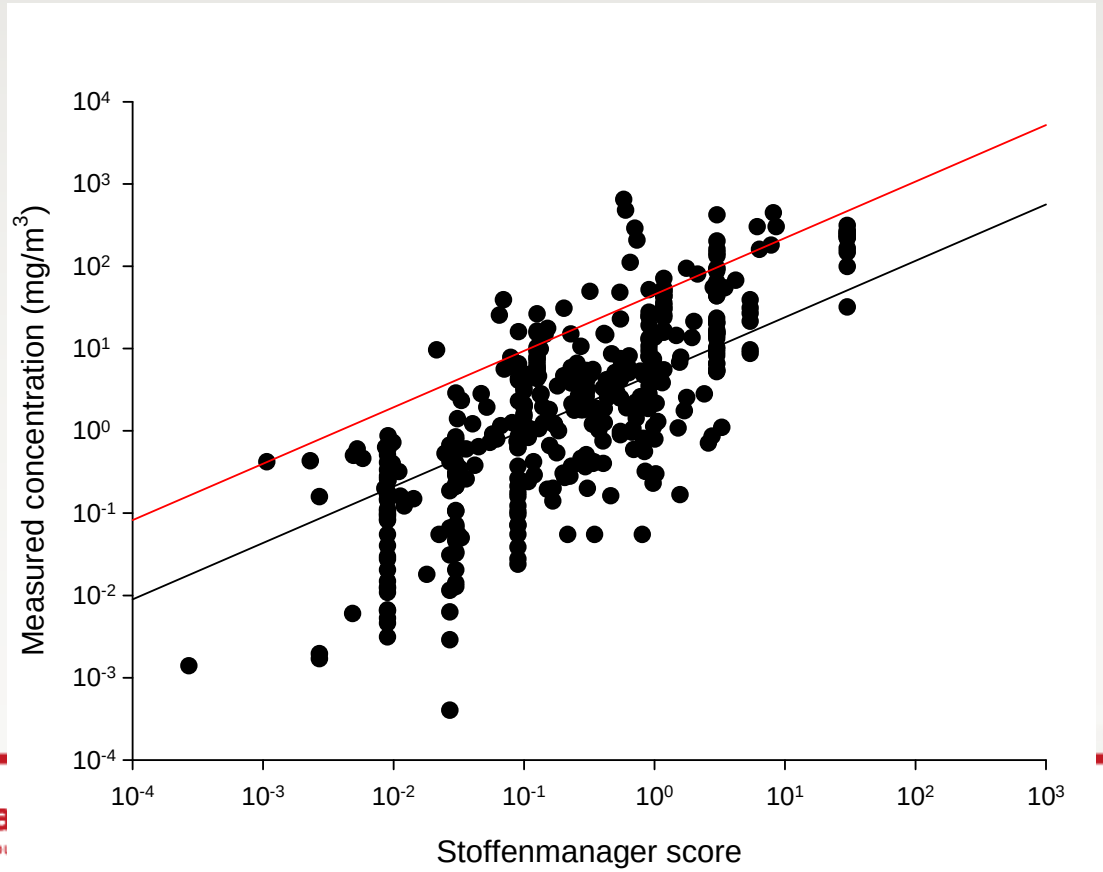
$$Score = \{[A * E] + [E * H * \eta \mathrm{lc\_nf} * \eta \mathrm{gv\_nf}] + [\mathrm{E} * \mathrm{H} * \eta \mathrm{lc\_ff} * \eta \mathrm{gv\_ff}]\} * \eta \mathrm{imm}$$

$$Score = \{[A * E] + [E * H * \eta \mathrm{lc\_nf} * \eta \mathrm{gv\_nf}]\} * \eta \mathrm{imm}$$

$$Score = \{[0.03 * 0.3] + [0.3 * 10 * 0.3 * 0.1]\} * 1 \ = \ 0.099$$

Stoffenmanager calibration

- This example was a good start of the calibration
  - 1 measurement with all the required contextual information
- More measurements were added
- Models were derived (median, 90th-percentile) to estimate exposures in (mg/m^3)



Cross-validation of the Stoffenmanager

- The validity of the predictions of any model should be evaluated before results can be used safely and effectively in the risk assessment process.
- Estimated exposure are compared with measured results in the validation dataset

	Calibration	Validation
Handling powders and granules	326	82
Handling resulting in communiting	52	60
Handling low-volatile substances	216	40
Handling volatile substances	104	72
Total number of measurements	698	254

Results cross-validation study

	N	r_s	Bias	Precision	Relative bias(%)	% > 90th percentile
Solid scenarios						
Handling of powders and granules	82	0.41	-1.49	1.66	-77	29
Handling resulting in comminuting	60	0.69	-0.10	1.71	-9	5
Liquid scenarios						
Low-volatile substances	40	0.20	-0.97	1.75	-62	15
Volatile substances	72	0.63	-0.11	1.61	-11	7

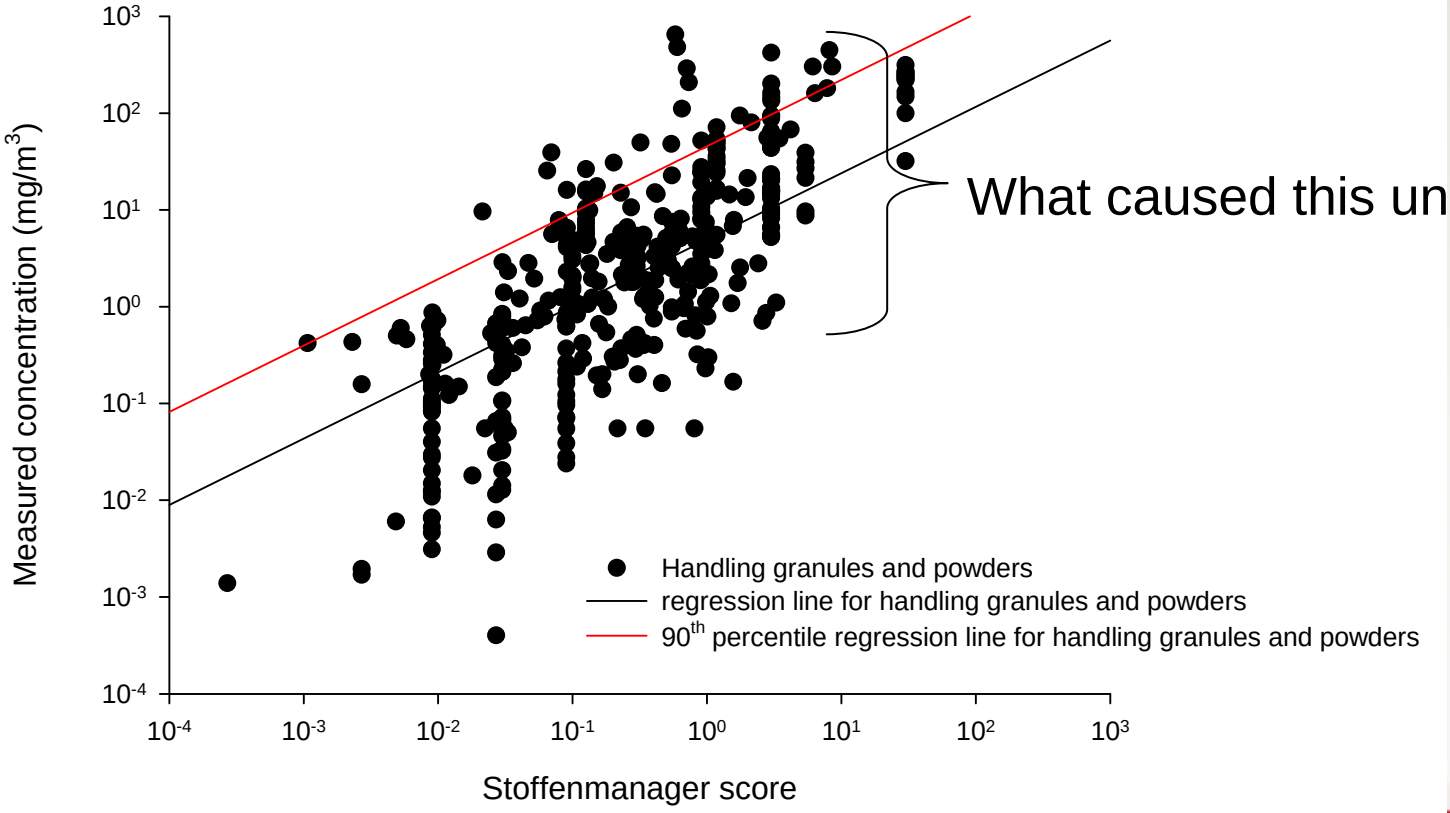
New models

	Calibration	Validation	New calibration
Handling powders and granules	326	82	408
Handling resulting in comminuting	52	60	112
Handling low-volatile substances	216	40	256
Handling volatile substances	104	72	176
Total number of measurements	698	254	952

- We derived 4 new models, these were validated again
- Validation of two solid scenarios in cooperation with BGIA
- More information?
- *Jody Schinkel, Wouter Fransman, Henri Heussen, Hans Marquart, Hans Kromhout and Erik Tielemans;* ***Cross-validation and refinement of the Stoffenmanager quantitative exposure algorithms.*** *Accepted OEM*

Discussion

- r_s =0.77 (n = 408)
- Explained variance 48%
- 52% unexplained
- Use 90th percentile model estimates as model outcome.



What caused this uncertainty?

Summary

- Stoffenmanager inhalation model is calibrated measured data
- The validity of the predictions were evaluated with measured data
- Results are publicly available for transparency
- 52% of variance remains unexplained

What causes this uncertainty?

- Uncertainty in measurement data
- Uncertainty in the model
- Uncertainty in input parameters

Discussion

- What could we do to increase the precision of the model?
- Reducing uncertainty in measurement data is not possible
- Model uncertainty could be decreased by:
  - Adding determinants
  - Assign more scientifically based scores
  - Review processes with experts
- Uncertainty in input parameters
  - We already used very strict requirements for the 1000 data points in this study.