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ART, Stoffenmanager (v4.0) and ECETOC TRAv3: a systematic comparison of the estimates

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Original Article

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ART, Stoffenmanager, and TRA: A Systematic Comparison of Exposure Estimates Using the TREXMO Translation System

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Abstract

Several occupational exposure models are recommended under the EU's REACH legislation. Due to limited availability of high-quality exposure data, their validation is an ongoing process. It was shown, however, that different models may calculate significantly different estimates and thus lead to potentially dangerous conclusions about chemical risk. In this paper, the between-model translation rules

Chemical exposure

Chemical exposure

- **Exposure measurements**
- Within- and between-worker variability
- Costs, time...
- Workers already exposed during the measurements

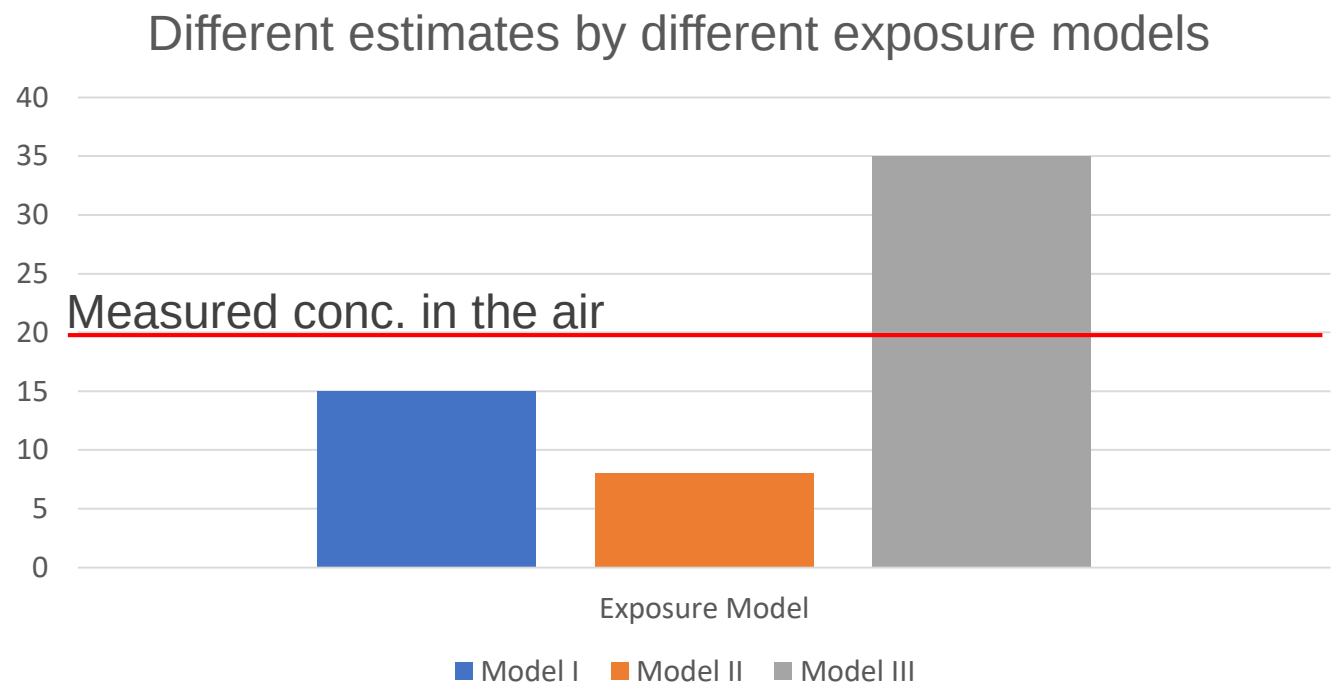
- **Exposure modeling**
- Simple mathematical algorithm
- Calibrated/validated against exposure data
- Cheap and fast alternative

REACH models

- **REACH** and **ChemO**
- Several models with different complexities
- Tier 1 and Tier 2

- **Advanced REACH Tool (ART)**
- **Stoffenmanager (SM)**
- **ECETOC TRA (TRA)**
- **...**

REACH models



- Small number of exposure measurements
- Unkown performances of the models
- Which model is the best for a given exposure situation?

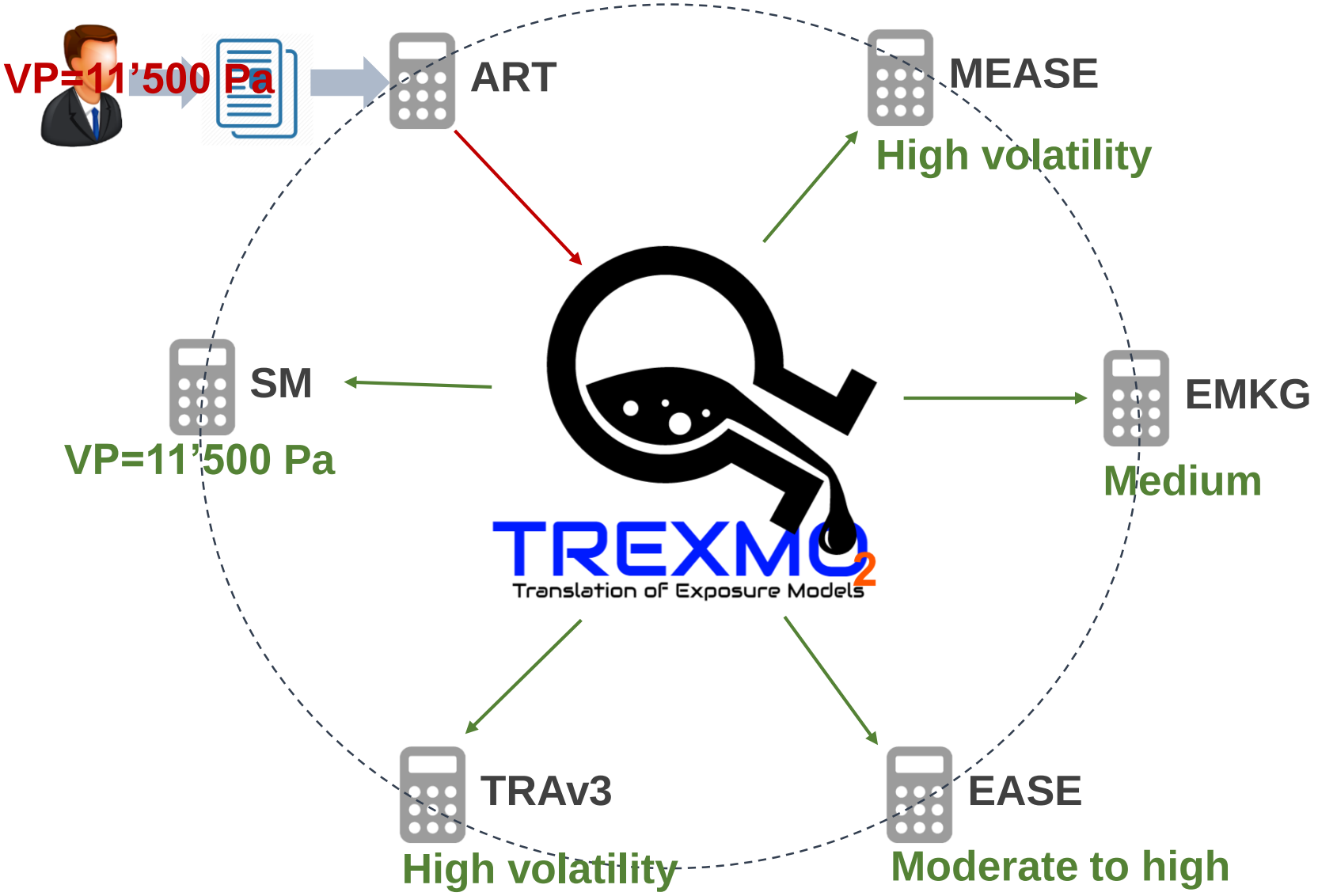
TREXMO

- A tool (not another model!) that includes six models:

    1. Advanced REACH Tool (ART)
    2. Stoffenmanager (v4.0)
    3. ECETOC TRAv3
    4. MEASE
    5. EMKG-EXPO-TOOL
    6. EASE 2.0

- **Inter-model translations**
- Multi models approach
- Between-user reliability

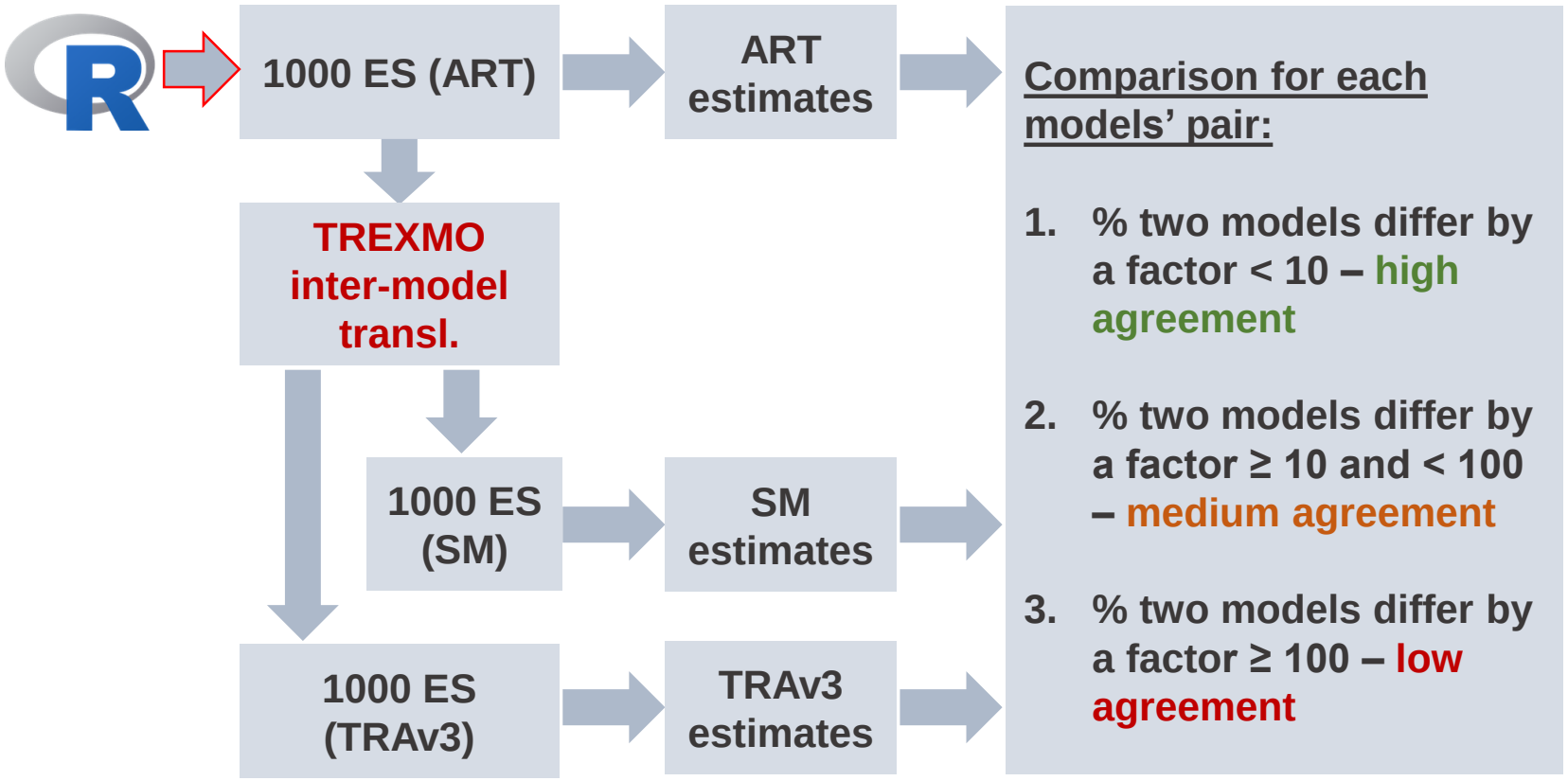
TREXMO


VP=11’500 Pa
ART
MEASE
High volatility
SM
VP=11’500 Pa
EMKG
Medium
TREXMO2
Translation of Exposure Models
TRAv3
High volatility
EASE
Moderate to high

Objective

- Evaluate differences between the estimates of ART, Stoffenmanager (v.4.0) and TRAv3 for all possible exposure conditions
- Determine how different exposure parameters and their combinations affect these differences

Methodology



- Each models' pair, i.e. **SM-ART**, **TRA-ART** and **TRA-SM**, analysed separately.
- The number of the generated ES increased until a next increment (1000 ES) changed the final results by less than 1%

Methodology

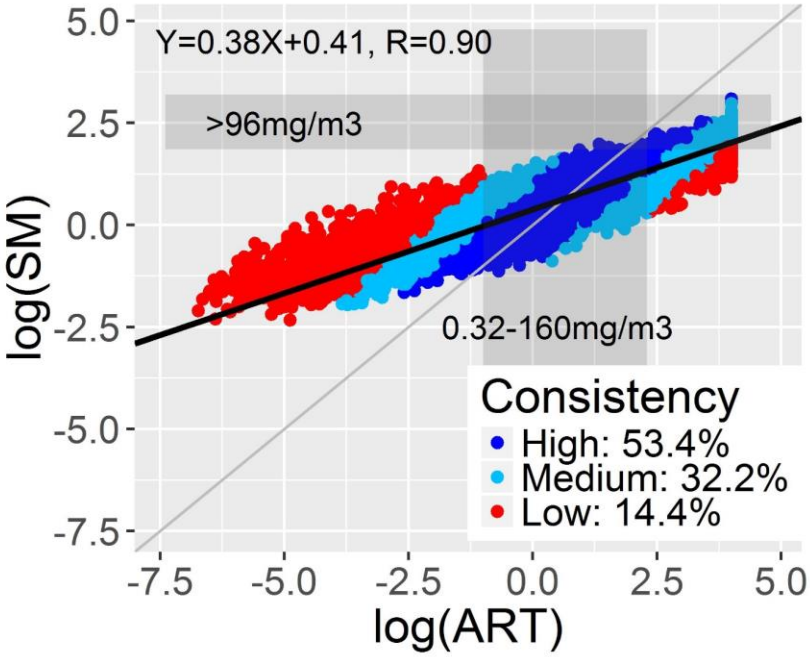
ES generated separately for:

1. liquids, dusts and solids
2. near- and far-field
3. indoors and outdoors

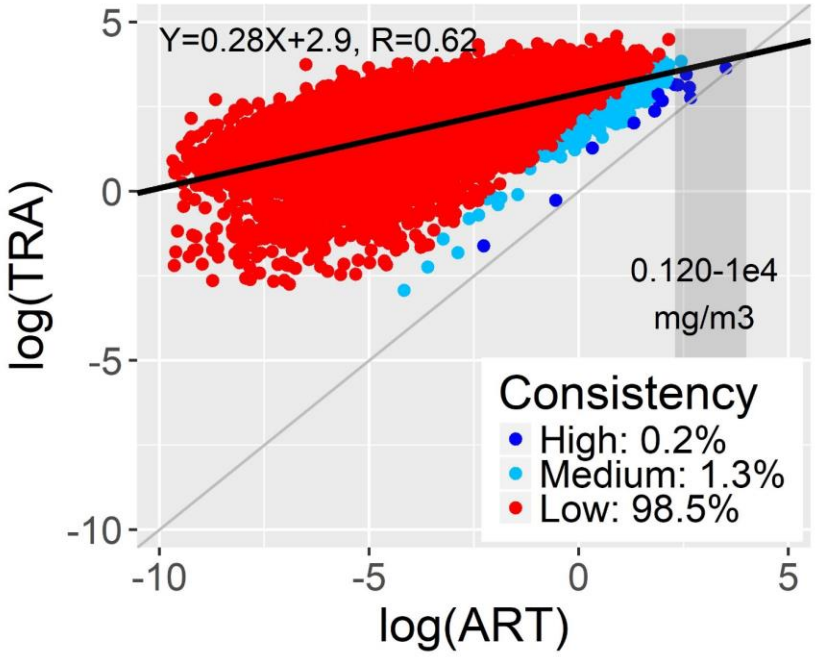
- Different exposure parameters used
- e.g. *segratation* not used for near-field exposure

Results

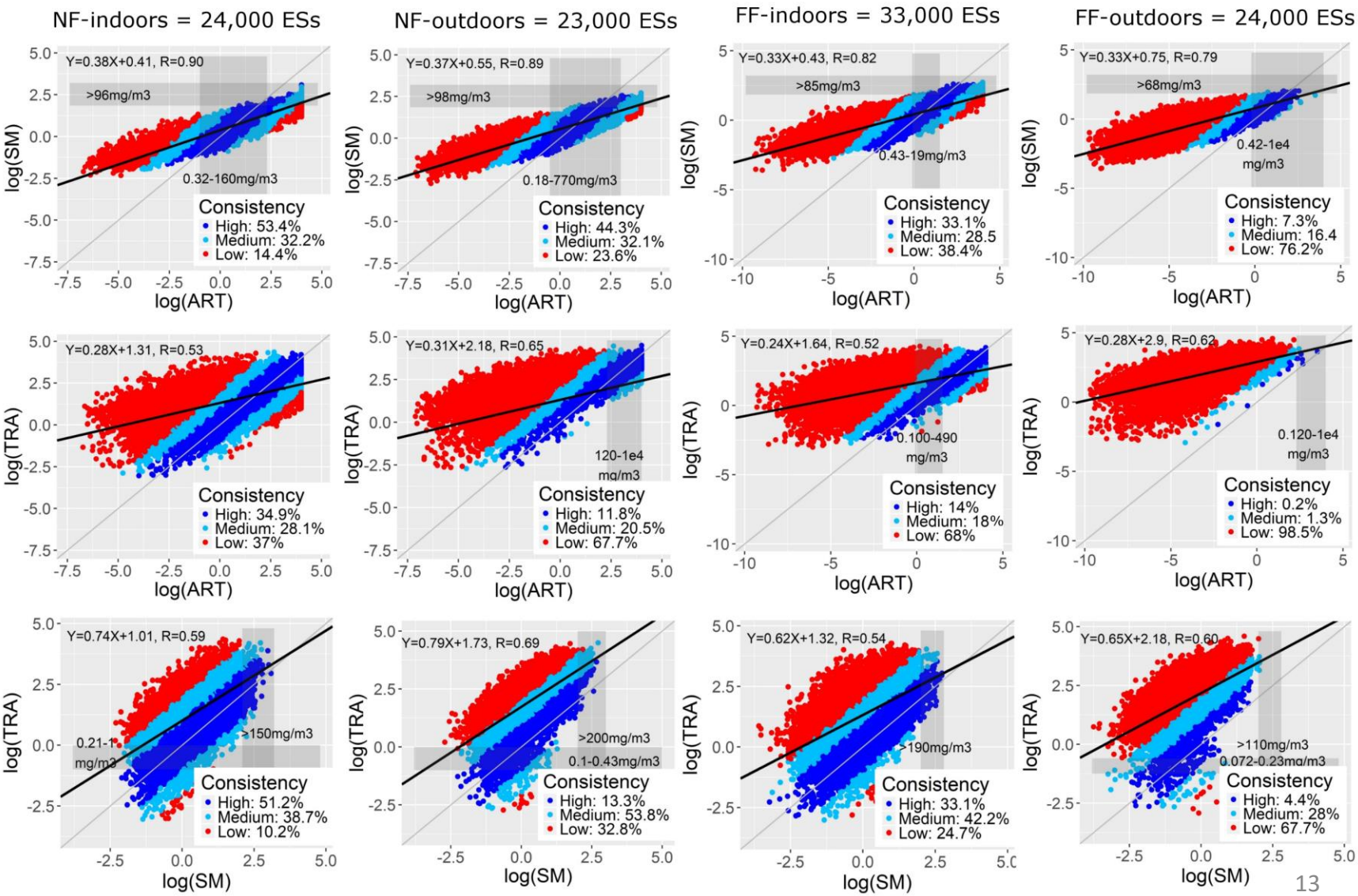
NF-indoors, 24 000 ES



FF-outdoors, 24 000 ES



Results


NF-indoors = 24,000 ESs
NF-outdoors = 23,000 ESs
FF-indoors = 33,000 ESs
FF-outdoors = 24,000 ESs
Y=0.38X+0.41, R=0.90
>96mg/m3
0.32-160mg/m3
Consistency
High: 53.4%
Medium: 32.2%
Low: 14.4%
Y=0.37X+0.55, R=0.89
>98mg/m3
0.18-770mg/m3
Consistency
High: 44.3%
Medium: 32.1%
Low: 23.6%
Y=0.33X+0.43, R=0.82
>85mg/m3
0.43-19mg/m3
Consistency
High: 33.1%
Medium: 28.5
Low: 38.4%
Y=0.33X+0.75, R=0.79
>68mg/m3
0.42-1e4
mg/m3
Consistency
High: 7.3%
Medium: 16.4
Low: 76.2%
log(SM)
log(ART)
Y=0.28X+1.31, R=0.53
Consistency
High: 34.9%
Medium: 28.1%
Low: 37%
Y=0.31X+2.18, R=0.65
120-1e4
mg/m3
Consistency
High: 11.8%
Medium: 20.5%
Low: 67.7%
Y=0.24X+1.64, R=0.52
0.100-490
mg/m3
Consistency
High: 14%
Medium: 18%
Low: 68%
Y=0.28X+2.9, R=0.62
0.120-1e4
mg/m3
Consistency
High: 0.2%
Medium: 1.3%
Low: 98.5%
log(TRA)
log(ART)
Y=0.74X+1.01, R=0.59
0.21-1
mg/m3
>150mg/m3
Consistency
High: 51.2%
Medium: 38.7%
Low: 10.2%
Y=0.79X+1.73, R=0.69
>200mg/m3
0.1-0.43mg/m3
Consistency
High: 13.3%
Medium: 53.8%
Low: 32.8%
Y=0.62X+1.32, R=0.54
>190mg/m3
Consistency
High: 33.1%
Medium: 42.2%
Low: 24.7%
Y=0.65X+2.18, R=0.60
>110mg/m3
0.072-0.23mg/m3
Consistency
High: 4.4%
Medium: 28%
Low: 67.7%
log(TRA)
log(SM)

Exposure parameters

- Multiple linear regression
- How much determinants and its parameters affect the models' difference

$$\log(m1) - \log(m2) = \beta_0 + \sum_{i=1} \beta_i \cdot \log d_i + \sum_{k=1} \beta_k \cdot d_k + \varepsilon$$

Estimate difference

Continuous parameters

Categorical parameters

- *How much VP determinant explains (affects) the difference?*
- *How the models' difference change with increase/decrease of VP?*

Exposure parameters

NF-indoors: contribution of ART determinants in explaining multiple R^2.

	Fug.	log(c)	Moist.	H	LC	Vol	ACH	Su	Multiple R^2
Vapours									
SM-ART	0.12	0.11		0.27	0.24	0.03	0.03	< 0.01	0.79
TRA-ART	0.11	0.09		0.14	0.32	0.03	< 0.01	< 0.01	0.70
TRA-SM	0.02	0.01		0.10	0.24	0.01	0.05	< 0.01	0.40
Dusts									
SM-ART	0.02	0.31	0.27	0.09	0.14	< 0.01	< 0.01	< 0.01	0.83
TRA-ART	0.02	0.07	0.19	0.08	0.26	0.01	< 0.01	< 0.01	0.65
TRA-SM	0.13	0.14	< 0.01	0.04	0.21	0.01	0.04	< 0.01	0.59
Solids									
SM-ART	0.03	0.44	0.22		0.16	< 0.01	< 0.01	< 0.01	0.86
TRA-ART	0.02	0.10	0.18		0.37	0.01	0.01	< 0.01	0.69
TRA-SM	< 0.01	0.23	< 0.01		0.36	0.03	0.07	< 0.01	0.69

Results (parameters)

Determinant	Parameters	SM-ART	TRA-ART	TR-SM
	Intercept	0.20	1.93	1.73
Vapour pressure (Pa)	log(P)	-0.46	-0.57	-0.12
Concentration (%)	log(c)	-0.46	-0.55	-0.09
Activity (sub)classes*	Surface spraying of liquids	0	0	0
	Spraying of liquids in a space	-0.39	-0.49	-0.09
	Activities with open surfaces undisturbed	1.03	0.41	-0.62
	Activities with open surfaces agitated	0.57	0.15	-0.42
	Handling of contaminated objects	1.43	0.65	-0.78
	Spreading of liquid products	0.96	0.97	0.01
	Application in high-speed processes	-0.03	-0.23	-0.20
	Transfer of liquids: bottom loading	1.43	1.31	-0.13
	Transfer of liquids: falling liquids	1.50	1.45	-0.05

Results (parameters)

Parameter combination:

VP = 1500 Pa

C = 100 %

Activity: *Spreading of liquid products*

LC: *Movable LEV*

Room volume: *100 m3*

General ventilation: *1ACH*

Increasing the VP, the difference increases in favour of ART

$$\log(\mathrm{SM}) - \log(\mathrm{ART}) = \beta_0 + \beta_{vp} \times \log(\mathrm{VP}) - \beta_c \times \log(\mathrm{c}) + \beta_a + \beta_{lc} + \beta_{vol} + \beta_{gv}$$

$$= 0.20 - 0.46 \times \log(1500) - 0.46 \times \log(100) + 0.96 + 0.04 + 0.14 + 0.04$$

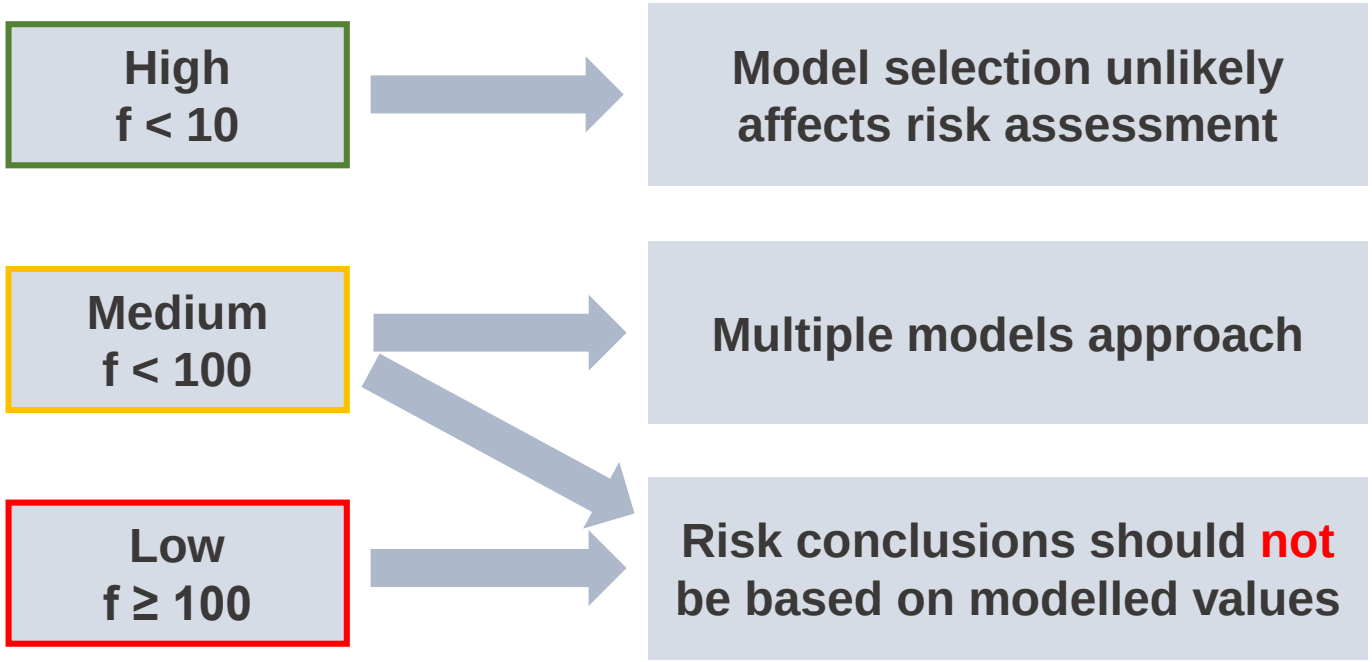
$$= -1$$

ART calculates an estimate by one order of magnitude higher than Stoffenmanager...

Conclusion

- Differences of few orders of magnitude
- ART (Tier 2) calculates often higher predictions with exposure parameters that describe higher exposure concentrations (e.g. high VP and conc, spraying etc)
- The tiered approach is not applicable always
- Different model - different risk conclusion
- Multiple model approach reasonable

Recommendation



Thank you for your attention!

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