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Title:

Stoffenmanager® algorithm within version 6 differs from the published algorithm within old versions and TREXMO

Authors:

Nenad Savic[1*], Bojan Gasic[2], David Vernez[1]

[1] Institute for Work and Health (IST), University of Lausanne and University of Geneva, Route de la Corniche 2, CH-1066 Epalinges-Lausanne, Switzerland

[2] Chemicals and Occupational Health Unit, Swiss State Secretariat for Economic Affairs (SECO), Holzikofenweg 36, CH-3003 Bern, Switzerland

[*]Author to whom correspondence should be addressed. Tel: (+41) 021 314 37 82. E-mail: nenad.savic@chuv.ch

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We appreciate the interest Dr. Heussen *et al.* have shown to the TREXMO tool (currently available at http://trexmo.unige.ch), which compares exposure estimates generated with six model algorithms. One of the models integrated in TREXMO is Stoffenmanager version 5.1.

In their letter to the editor, Heussen *et al.* put forth two claims; The first being that significant differences in exposure estimates calculated for Stoffenmanager using TREXMO and their new commercial Stoffenmanager® version 6 are observed; and second, that TREXMO cannot contribute much to the between-user reliability.

As we clearly stated in our paper, TREXMO includes Stoffenmanager version 5.1's algorithm published in the Annals of occupational hygiene in 2009 (Schinkel *et al.*, 2009). Changes implemented in the current commercial version of Stoffenmanager® version 6 were not considered, as these algorithms have never been published in a peer-reviewed journal. Stoffenmanager version 6 algorithm is unknown to the TREXMO authors and also to the downstream users. So, comparing the estimates from Stoffenmanager® version 6 with TREXMO, is in effect testing their own updated version's algorithm – not detecting errors in the TREXMO algorithm. Heussen et al.'s claim that TREXMO contains error on that basis is therefore unsupported and possibly misleading for the readers.

Updates in the version 6.0, currently available on Stoffenmanager's official web-page, can explain the differences shown by Heussen *et al*. Besides, in Dr. Heussen's examples, the results were only given for the 90th percentile, which might have enlarged the absolute differences. The 50th percentile, which is the direct output of the score calibration, was however omitted.

Due to the reaction of Dr. Heussen, the differences between TREXMO, Stoffenmanager® version 6 and the published algorithm (Schinkel *et al.,* 2009) were further investigated for a set of exposure situations. The estimates were also calculated manually using the scoring system (Marquart *et al.,* 2008) and the refined calibration in Schinkel *et al.* (2009). Twenty-six semi-random exposure situations including exposure to dust, abrasive dust (solid) and liquid were established and the corresponding estimates calculated. An exposure situation was generated for each "handling type" defined in Stoffenmanager, while the other exposure parameters were randomly selected. The results are shown in Tables 1-3. The differences found were insignificant (< 0.1%) between the estimates calculated in TREXMO and manually using the published data of Schinkel *et al.,* (2009). However, differences between Stoffenmanager® version 6 and the published algorithm were found. These results suggest that the new version of Stoffenmanager® uses an updated algorithm and/or calibration parameters. Considering that these updates have not been published, the new version can hardly be used as "gold standard" to verify the algorithm used in TREXMO. We therefore consider Heussen *et al.*'s claim that TREXMO contains error unsupported and possibly misleading for the readers.

While performing this comparison, we have noticed that, in Stoffenmanager® version 6, the so-called "immission" (see Marquart *et al.* 2008) exposure factor is now available for selection also for near-field exposure situations. This factor addresses situations where the worker uses cabins or performs a task in a room separated from the primary exposure source. In our opinion, it should be only considered for far-field exposure situations. This might be a technical mistake in the Stoffenmanager® version 6 and should be reviewed.

Heussen *et al.* also commented on a few parameter text descriptors used in TREXMO and compared it to the new version of Stoffenmanager®. Once again, the TREXMO uses the identical text descriptors as were given in the published versions (see Marquart *et al.* 2008 and Schinkel *et al.* 2009). However, one text descriptor in our tool and addressed by

Heussen *et al.* contained a syntax error and was corrected accordingly: “handling of liquids using pressure, low speed and medium sized enterprises” to “handling of liquids using low pressure, low speed and medium sized surfaces” and “handling of products in very small amount or in situation where only low quantities of product are likely to be released” to “handling of products in small amount or in situation where only low quantities of product are likely to be released”. We thank Heussen *et al.* for identifying the two typos.

About between user variability

The between-user reliability issue was also brought up in Heussen *et al.*’s letter to the editor. One of TREXMO’s main goals is to act as an algorithm “translator” and thus reduce the between-user variability, which likely occurs when using exposure models. We fail to understand Heussen *et al.*’s argument here. We agree that TREXMO cannot reduce the variability of the initial assessment (starting model), when coding the exposure situation into a model for the first time. The variability in translating the exposure situation further into the other models using TREXMO, is however expected to be lower than the obtained when coding the exposure situation “manually” into another model. However, the reduction of the between-user variability brought by TREXMO must be validated. The Institute for Work and Health in collaboration with international experts conducted a study to show how the TREXMO affect this variability. These results will be submitted for publication in the forthcoming months. The translation system used in TREXMO has however already be validated through a review by external experts prior to the publication (Savic *et al.,* 2016).

It is the goal of TREXMO to encourage assessors to use multiple modelling approaches instead of selecting a single model, in order to support a more robust assessment. Little is known regarding actual performance of the different models and their relative domain of validity. Selecting *a priori*, which model is the most adequate is therefore tricky. Using a multiple model approach to know which model is the most conservative and whether the results between models are consistent is of key importance. So, rather than encouraging using of the most favourable model estimate, as alleged, by Heussen *et al*., which is already possible nowadays, TREXMO supports a better decision making by giving an extended perspective of the results (Riedmann *et al.,* 2015). It is our belief that the vast majority of the assessors are interested in making the best estimate. Giving them the opportunity to compare several outcomes rather than using a single model’s results seems appropriate in that regard.

Current development status and future versions

The TREXMO version online is still a testing version (as stated on its home page), not the final end-user version. TREXMO is now referenced by the European Chemical Agency (ECHA) in the updated guidance on exposure assessment (chapter R.14, ECHA 2016). Many positive comments and suggestions have been received, and are currently being used to improve the tool. The next version, TREXMO 1.5, is already under development and will incorporate a friendlier user interface. This version will be the first end-user version.

Conclusion

As errors are always possible, we welcome feedbacks and will make our best efforts in improving TREXMO. So far, however, no significant discrepancy has been found between the original Stoffenmanager version 5.1 model and TREXMO’s results nor to other models. It appears that Heussen et al.’s claims that TREXMO has incorporated Stoffenmanager erroneously are unsupported.

Stoffenmanager version 6 was updated; however, the coding for this has not been made publicly available. If the latest changes in the version 6 would be published in a peer-reviewed journal then we could integrate these changes into TREXMO.

TREXMO is a non-profit tool, freely available to the exposure assessors. It aims to improve the exposure assessment practices and ultimately, improve health protection. This scientific and systematic approach comparing publicly available exposure tools bears no commercial intent and should not be put into competition with Stoffenmanager® 6.

Table 1. Exposure estimates (in mg/m^3), at the 50th and the 90th percentile, calculated with TREXMO, with the algorithm in Schinkel *et al.* (2009) and with Stoffenmanager version 6.0 for situations corresponding to exposure to dust. The absolute and relative differences between TREXMO - Schinkel and Stoffenmanager version 6 - Schinkel are presented.

Exposure Situation	TREXMO		Schinkel et al., 2009		Stoffenmanager v.6		TREXMO vs Schinkel		Stoffenmanager v.6 vs Schinkel	
	50th	90th	50th	90th	50th	90th	Absolute dif.	Relative dif.	Absolute dif.	Relative dif.
1	253.56	2336.31	253.56	2336.28	247.00	2272.00	0.00	0.00	-6.56	-2.59
2	51.77	477.01	51.77	477.00	50.93	469.00	0.00	0.00	-0.84	-1.62
3	2.16	19.89	2.16	19.90	2.18	20.07	0.00	0.00	0.02	0.93
4	0.09	0.83	0.09	0.83	0.10	0.91	0.00	0.00	0.01	8.89
5	0.19	1.77	0.19	1.75	0.21	1.92	0.00	0.00	0.02	10.53
6	1.08	9.95	1.08	9.95	1.28	11.82	0.00	0.00	0.20	18.52
7	0.44	4.06	0.44	4.05	0.72	6.61	0.00	0.00	0.28	63.64
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 2. Exposure estimates (in mg/m^3), at the 50th and the 90th percentile, calculated with TREXMO, with the algorithm in Schinkel *et al.* (2009) and with Stoffenmanager version 6.0 for situations corresponding to exposure to abrasive dust. The absolute and relative differences between TREXMO - Schinkel and Stoffenmanager version 6 - Schinkel are presented.

Exposure Situation	TREXMO		Schinkel et al., 2009		Stoffenmanager v.6		TREXMO vs Schinkel		Stoffenmanager v.6 vs Schinkel	
	50th	90th	50th	90th	50th	90th	Absolute dif.	Relative dif.	Absolute dif.	Relative dif.
1	125.09	842.34	125.10	842.41	127.00	859.00	-0.01	-0.01	1.90	1.50
2	3.44	23.20	3.44	23.16	3.45	23.29	0.00	0.00	0.01	0.29
3	0.57	3.85	0.57	3.84	0.61	4.13	0.00	0.00	0.04	6.56
4	8.81	59.33	8.81	59.33	8.87	59.96	0.00	0.00	0.06	0.68
5	214.78	1446.30	214.77	1446.24	219.00	1479.00	0.01	0.00	4.23	1.93
6	91.17	613.91	91.16	613.86	92.55	253.00	0.01	0.01	1.39	1.50
7	35.64	240.03	35.64	240.00	36.05	244.00	0.00	0.00	0.41	1.14
8	15.13	101.88	15.13	101.88	15.26	103.00	0.00	0.00	0.13	0.85
9	0.61	4.14	0.61	4.14	0.61	4.14	0.00	0.00	0.00	0.00
10	0.16	1.10	0.16	1.40	0.16	1.09	0.00	0.00	0.01	0.71

Table 3. Exposure estimates (in mg/m^3), at the 50th and the 90th percentile, calculated with TREXMO, with the algorithm in Schinkel *et al.* (2009) and with Stoffenmanager version 6.0 for situations corresponding to exposure to vapours. The absolute and relative differences between TREXMO - Schinkel and Stoffenmanager version 6 - Schinkel are presented.

Exposure Situation	TREXMO		Schinkel et al., 2009		Stoffenmanager v.6		TREXMO vs Schinkel		Stoffenmanager v.6 vs Schinkel	
	50th	90th	50th	90th	50th	90th	Absolute dif.	Relative dif.	Absolute dif.	Relative dif.
1	1310.19	11812.91	1310.84	11812.28	1307.00	11801.00	-0.65	-0.05	-3.84	-0.29
2	692.54	6240.67	692.54	6240.64	690.00	6230.00	0.00	0.00	-2.54	-0.37
3	479.62	4322.00	479.62	4321.97	478.00	4313.00	0.00	0.00	-1.62	-0.34
4	267.93	2414.41	267.94	2414.47	267.00	2408.00	-0.01	0.00	-0.94	-0.35
5	141.55	1275.51	141.55	1275.54	141.00	1271.00	0.00	0.00	-0.55	-0.39
6	5.25	47.34	5.25	47.31	5.21	47.00	0.00	0.00	-0.04	-0.76
7	2.78	25.01	2.78	25.05	2.75	24.46	0.00	0.00	-0.03	-1.08
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

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