

VERMEER FCM: a tool combining migration modelling and in silico hazard predictions for substances migrating from food contact materials

Commonly used acronym: VERMEER FCM

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Organisation

Name of the organisation Sciensano

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SCOPE OF THE METHOD

The Method relates to	Human health
The Method is situated in	Regulatory use - Routine production, Translational - Applied Research
Type of method	In silico

DESCRIPTION

Method keywords

QSAR
quantitative property-property relationships
hazard
migration

Scientific area keywords

food contact material
in silico models
migration modelling
hazard assessment
plastic packaging

Method description

For the risk assessment of compounds migrating from food contact materials (FCM), information on the exposure to the migrant as well as its possible hazards is needed. To support the evaluation of both starting products and NIAS from plastic FCM, the VERMEER FCM tool has been developed within the context of the European Life VERMEER project (ENV/IT/000167). The software, freely available, is integrated in MERLIN-Expo and has been designed in line with the regulatory framework for plastics FCM. VERMEER FCM consists of 3 modules that allow (i) to model the migration of

chemicals into food, (ii) to predict toxicological endpoints relevant for FCM compounds and (iii) to automatically check whether the compound of interest is included in the positive list of the European Regulation on plastic FCM 10/2011. The three modules can be run either separately or in combination. The migration model integrated in VERMEER FCM has been newly developed and allows to run both deterministic and probabilistic simulations. Hazards are predicted by QSAR models that have been selected from the publicly available VegaHUB and include models for genotoxicity, subchronic toxicity, reproductive and developmental toxicity as well as carcinogenicity. In order to apply the VERMEER FCM tool, users are asked to provide information regarding the chemical(s) of interest (including the SMILES formula), the FCM and the food concerned, and other important parameters such as the contact time between food and FCM, contact temperature and some physico-chemical properties of the chemical migrant.

Lab equipment

Computer: the software can be freely downloaded via <https://www.vegahub.eu/portfolio-item/vermeer-fcm/>.

Method status

Internally validated

PROS, CONS & FUTURE POTENTIAL

Advantages

(Q)SAR models are time-, cost- and animal-saving in nature. Moreover, the VERMEER FCM tool is freely available via <https://www.vegahub.eu/portfolio-item/vermeer-fcm/>.

Challenges

- The QSAR results combine the prediction with the applicability domain index value. For a good interpretation the results have to be interpreted together with their associated reliability which is a unique feature for VEGA models.
- The tool combines migration modelling and hazard predictions by QSAR models to support the risk assessment of substances migrating from food contact materials. Migration data have to be combined with consumption data to obtain exposure estimates.

Modifications

Currently, the VERMEER FCM tool focuses on plastic FCM but in the future, it will be extended to other FCM materials.

Future & Other applications

The tool can also be applied to cosmetic plastic packaging. In the future, additional hazard models can be included.

REFERENCES, ASSOCIATED DOCUMENTS AND OTHER INFORMATION

References

User guide available via <https://www.life-vermeer.eu>
<https://doi.org/10.1016/j.fct.2024.115059>

Links

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