

# FCM MIGRATION MODELLING

## REQUEST FOR DATA



The European Reference Laboratory for food contact materials (EURL-FCM) developed a guideline for modelling the migration of substances from plastic materials (polymers) into food or food simulants.<sup>1</sup> In the meantime several software programs have been developed such as Migratest<sup>2</sup>, migraSIM/migraDASH<sup>3</sup>, SML<sup>4</sup>, SPFF<sup>5</sup>, VERMEER FCM<sup>6</sup>. There is a need for data to expand the applicability of the current guideline and to perform validation of existing estimation procedures for parameters like diffusion and partition coefficients in support of diffusion models. The data for estimation of diffusion coefficients for a specific plastic material (polymer) are typically data from kinetic experiments meaning the determination of the migration of several substances at combinations of different temperatures and different contact times from the plastic material (polymer) under consideration. Migration data on different substances are needed to cover a range of molecular weights. Migration data at different temperatures and contact times are needed to cover the various possible intended uses of the selected plastic material.

If you have such kinetic data and you intend to share them, please fill in for each type of plastic FCM separately the parameters below and send the form to [JRC-EURL-FCM@ec.europa.eu](mailto:JRC-EURL-FCM@ec.europa.eu).

## FCM Parameters

*The mandatory parameters are highlighted in bold. If you have done kinetics with a multi-layer plastic, please give information on the nature of each FCM layer (up to the absolute barrier if present).*

Nature of the plastic FCM	
<b>Type of polymer as specific as possible</b>	
<b>Migration test conditions</b> <ul style="list-style-type: none"><li>• <b>Temperatures (T; °C)</b></li><li>• <b>Contact times (t; min, h, day)</b></li></ul>	
<b>Contact area between FCM and Food (A) during the migration test performed (dm<sup>2</sup>)</b>	
<b>Density of FCM (<math>\rho_P</math>; kg/L)</b>	
<b>Thickness of the FCM layer (d)</b>	
Specific contribution of the FCM to the diffusion activation energy ( $\tau$ ) <i>(only if determined)</i>	
Polymer-specific constant ( $A_p^*$ ) <i>(only if determined)</i>	
FCM-Food partition coefficient (K) <i>(only if determined)</i>	

<sup>1</sup> Brandsch R, Dequatre C, Mercea P, Milana M, Stoermer A, Trier X, Vitrac O, Schaefer A and Simoneau C. Practical guidelines on the application of migration modelling for the estimation of specific migration. EUR 27529. Luxembourg (Luxembourg): Publications Office of the European Union; 2015. JRC98028. (Available on <https://publications.jrc.ec.europa.eu/repository/handle/JRC98028>)

<sup>2</sup> <https://www.fabes-online.de/software/>

<sup>3</sup> <https://saferithm.com/>

<sup>4</sup> [https://www.akts.com/sml/specific-migration-limits-diffusion-migration-multilayer-packaging-short-description/?doing\\_wp\\_cron=1681818989.3006141185760498046875](https://www.akts.com/sml/specific-migration-limits-diffusion-migration-multilayer-packaging-short-description/?doing_wp_cron=1681818989.3006141185760498046875)

<sup>5</sup> <http://sfpp3.agroparistech.fr/>

<sup>6</sup> <https://www.vegahub.eu/portfolio-item/vermeer-fcm/>

## Food/food simulant parameters

The mandatory parameters are highlighted in bold.

Description of the food/food simulant	
Type of food /food simulant	
Volume of the food/food simulant (V) during the migration test performed (dm <sup>3</sup> )	
Density of the food ( $\rho_F$ )	

## Chemical parameters

The mandatory parameters are highlighted in bold.

Description of the substance	
List of the substance(s)	
CAS No. for each substance ( <i>if available</i> )	
SMILES for each substance	
Molecular weight (M; Da) for each substance	
Initial concentration for each substance in the FCM (C <sub>i</sub> ; mg/kg polymer)	
Diffusion coefficient for each substance in FCM (DF; cm <sup>2</sup> /s)	
Octanol-water coefficient (in log <sub>10</sub> ) ( <i>only if available</i> )	
Migration result for each substance (M; mg/kg food)	

Please add the reference if relevant such as publication or report:

### Your contact details:

Name	
Organisation	
Address	
Country	
Email	
Phone	

