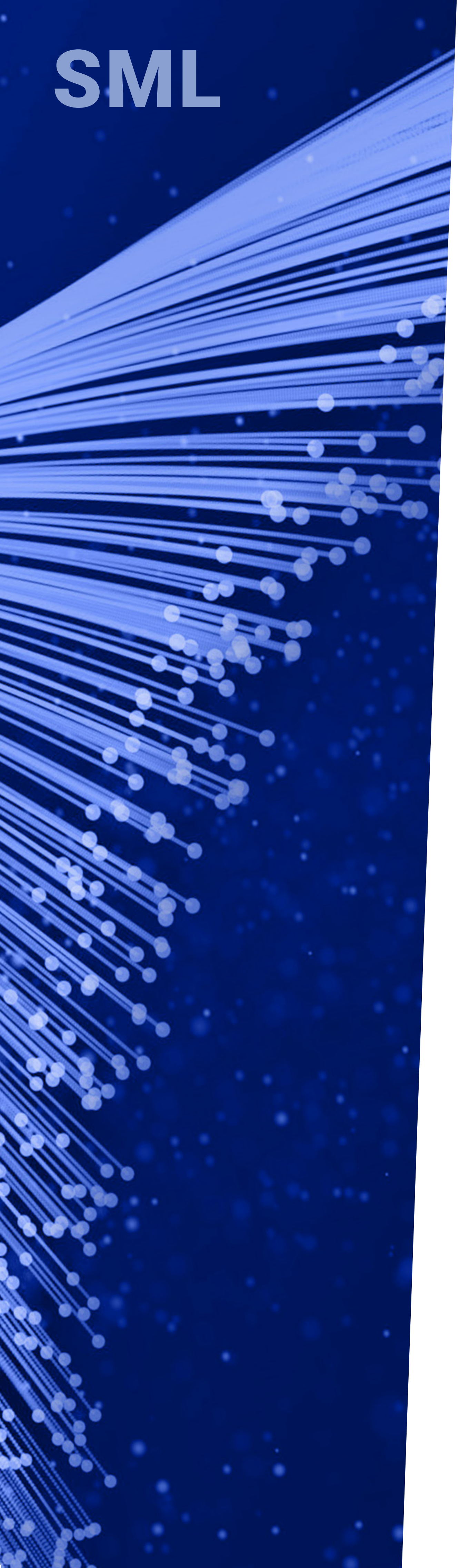


SPECIFIC MIGRATION LIMITS Software (SML)

Prediction of Migration Rate of Species from Packaging Materials to Packed Goods

CONTENT

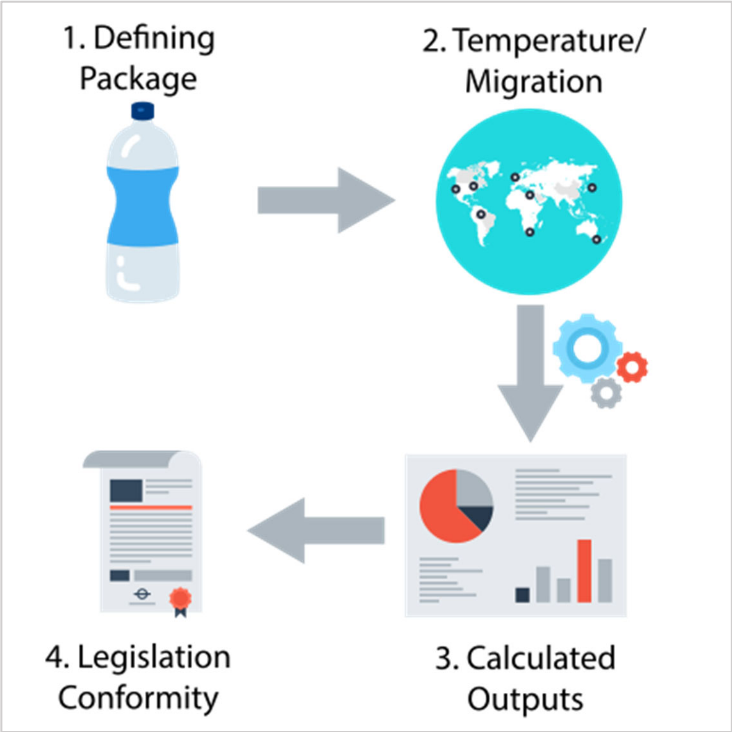
AKTS E-Learning

www.akts.com/sml/e-learning

TABLE OF CONTENTS

The **SPECIFIC MIGRATION LIMITS Software (SML)** allows the specific migration assessment for complex materials with different geometries and any multi-layer structure. Simulation of the migration process is based on Fick's 2nd law of diffusion under consideration of partitioning between adjacent layers or contact media in closed systems. The software contains a database of more than 20'000 chemicals and offers comprehensive estimation procedures for diffusion and partitioning coefficients. In case of missing required parameters, the software marks the method in red and indicates which parameters are missing. The end-user can add these parameters manually (if known) or has to choose another method.

The use of SPECIFIC MIGRATION LIMITS Software (SML) can proceed in four steps:



The workflow has therefore four main steps:

1. Define the package by creating the different articles of the package and introduce their properties.
2. Predict the migration using different temperature profiles (iso, non-iso, worldwide climate, etc.).
3. Analyse the calculated outputs.
4. Check the conformity of the results with corresponding legislations.

PACKAGE STRUCTURE

A package is a group of different articles, each having different layers properties. For instance, a bottle can be treated as two articles: the bottle cap and the bottle body. An article is composed of one or more layers of different sizes and properties.

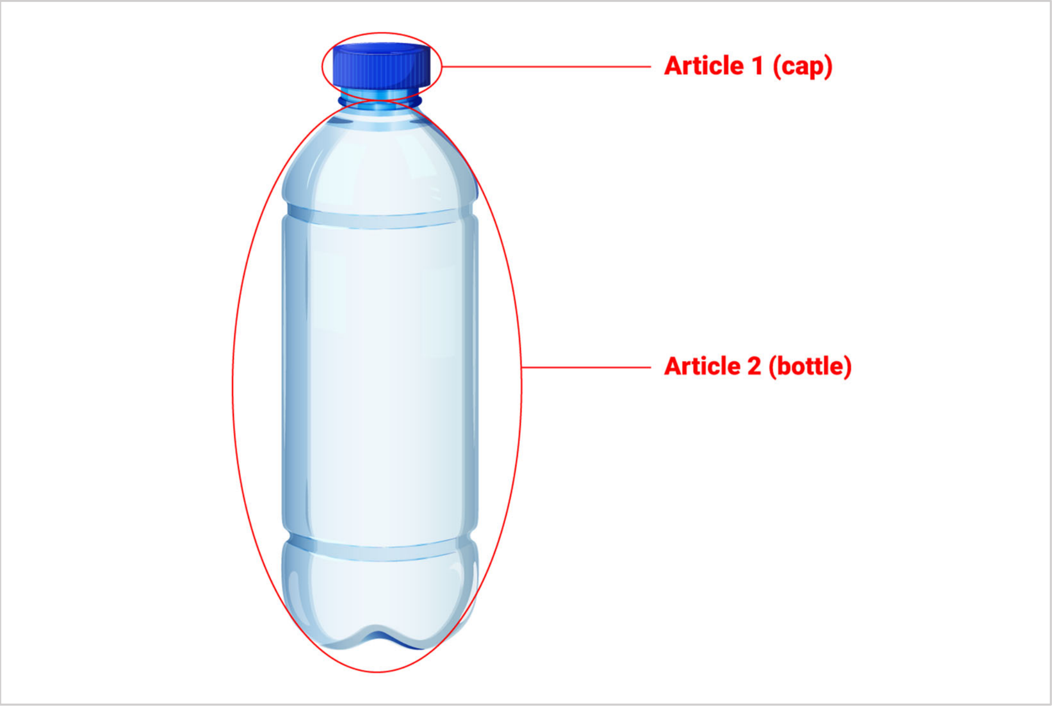


FIG. 1 - A package can be composed of multiple articles.

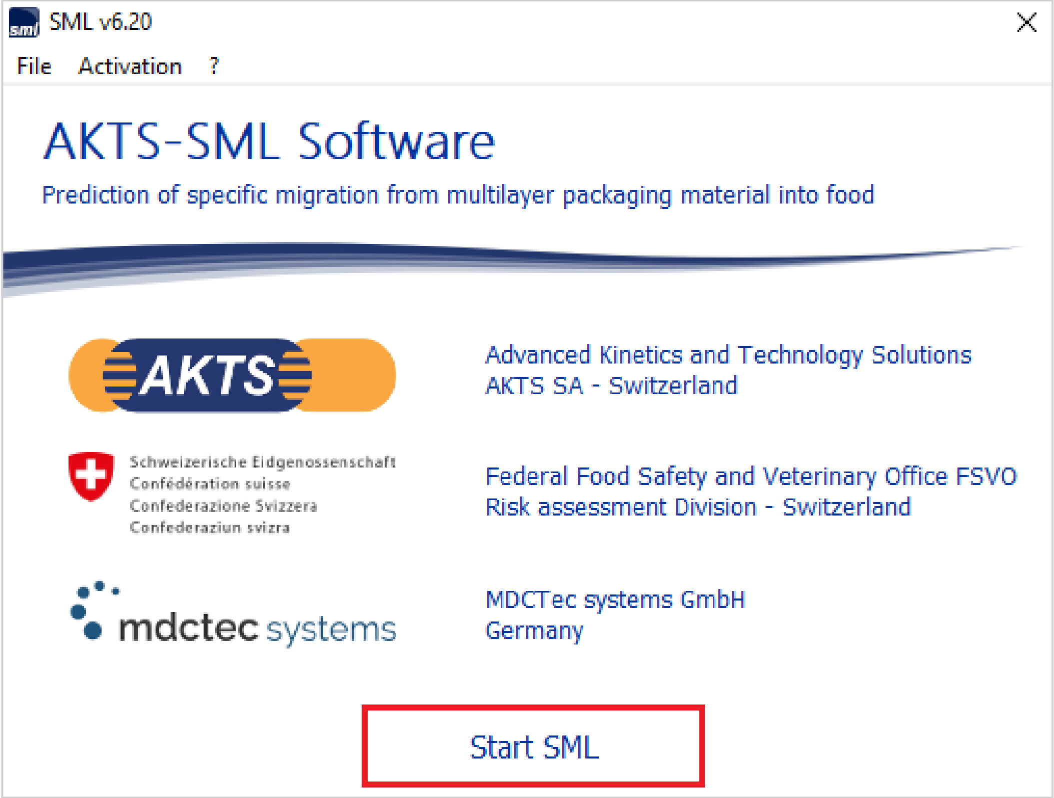


FIG. 2 - Click on 'Start SML' to start the work with the software.

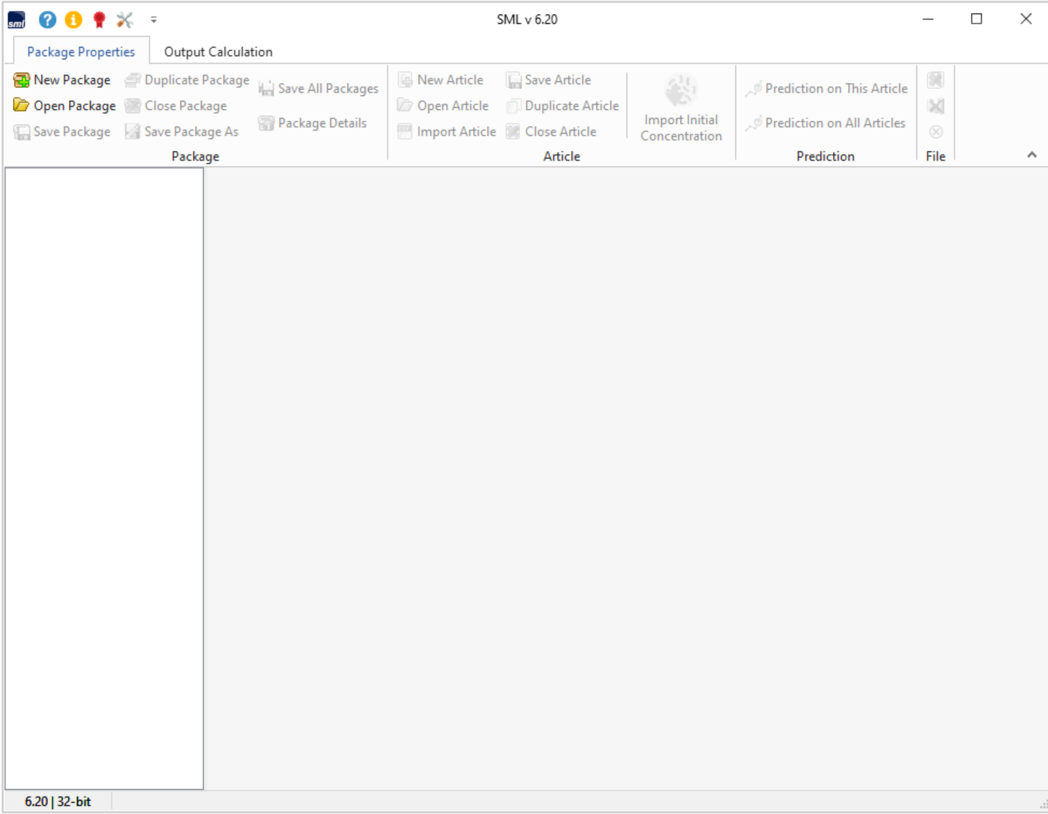


FIG. 3 - Opening screen of SML

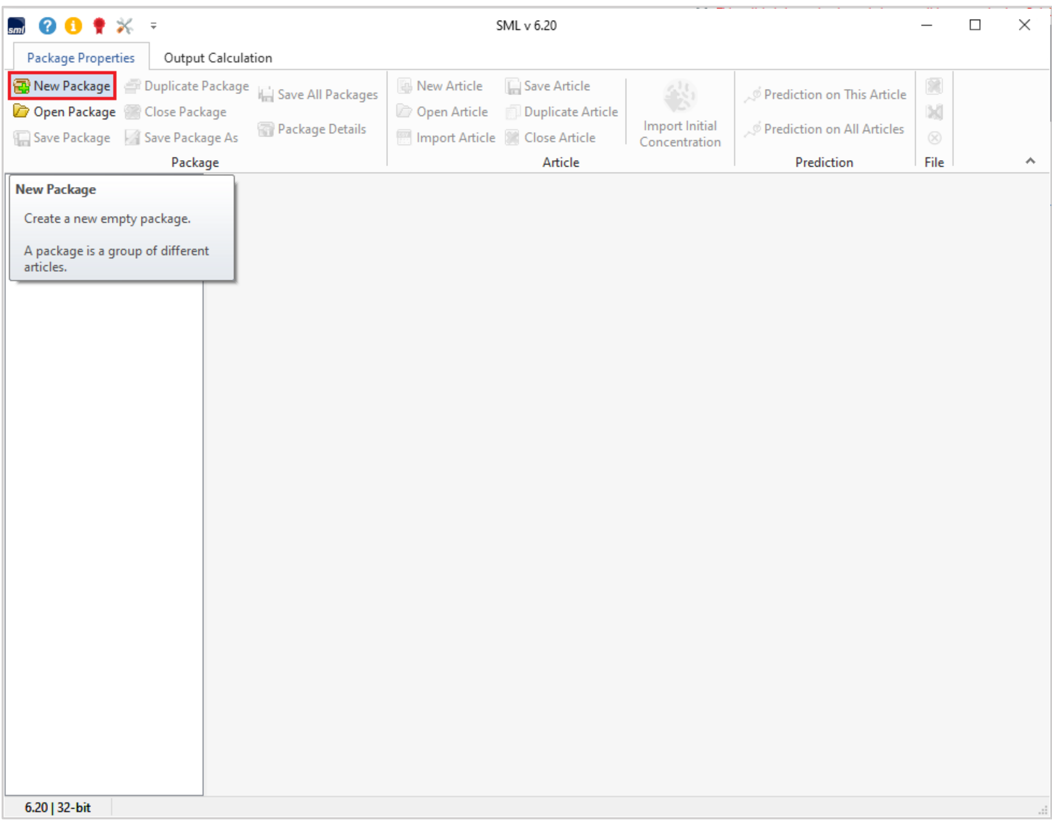


FIG. 4 - Selection of a new package.

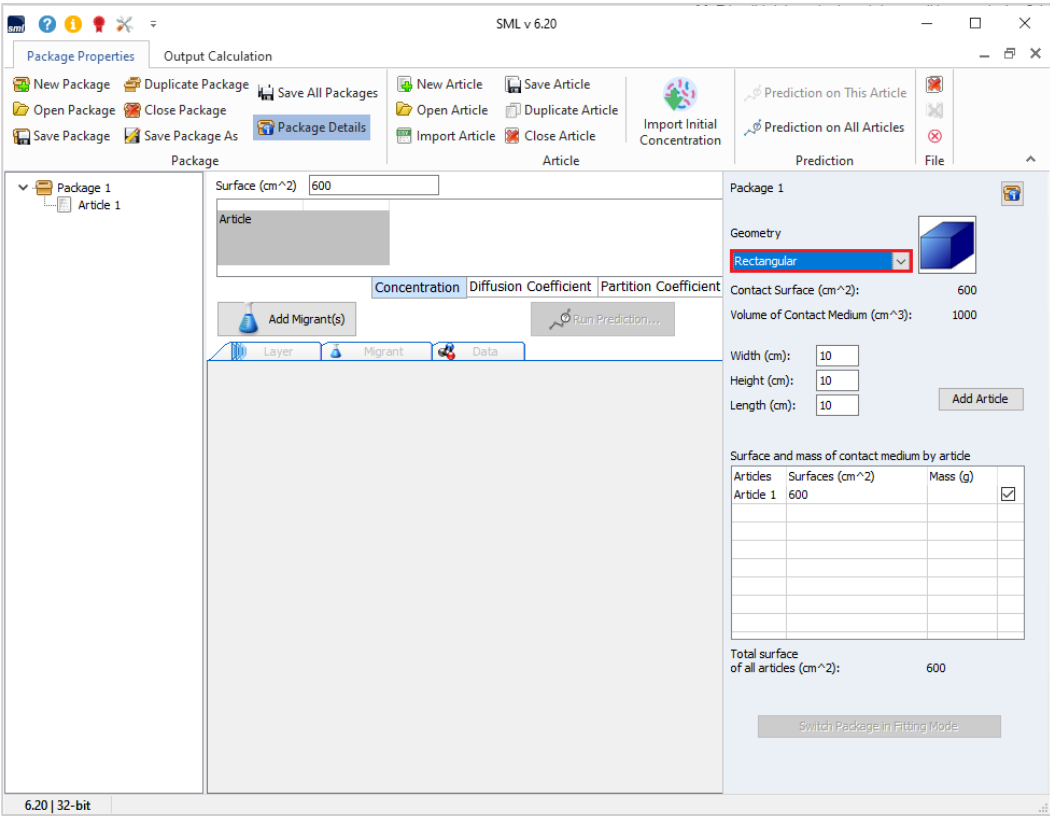


FIG. 5 - Selection of the package geometry (e.g. rectangular).

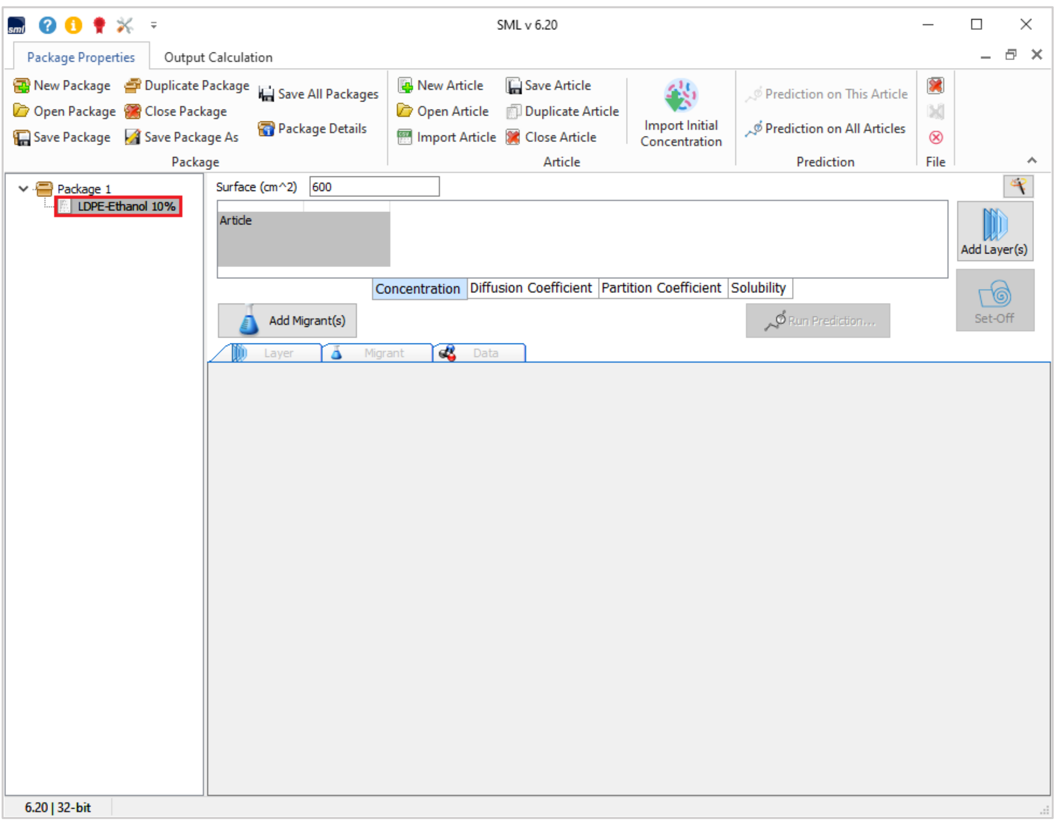


FIG. 6 – The package can contain one or more articles (e.g. bottle body and its lid).

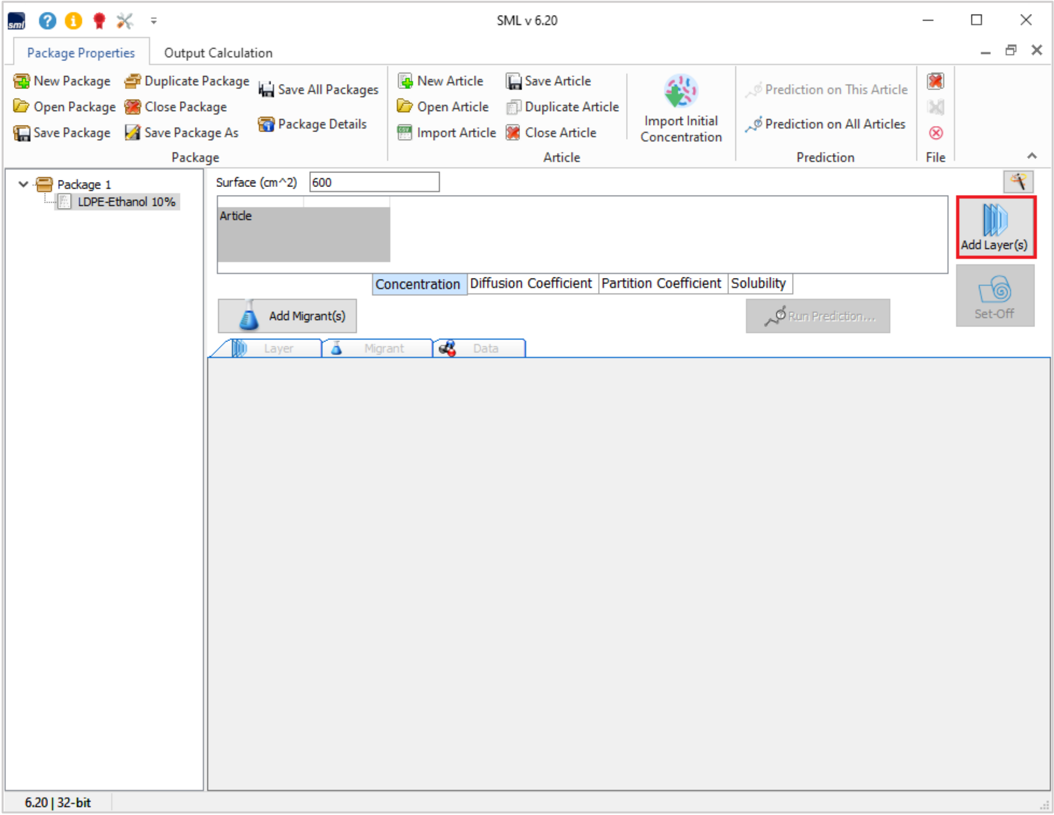


FIG. 7 - Construction of an article by adding layers.

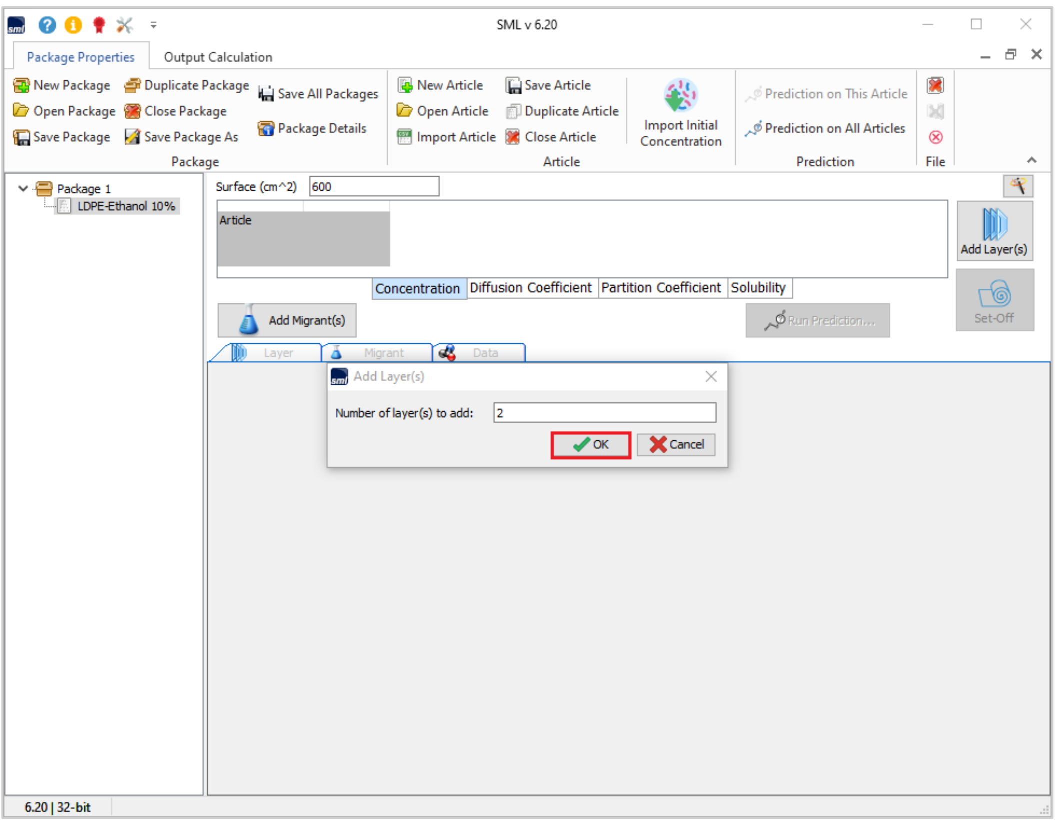


FIG. 8 - Introducing a number of layers.

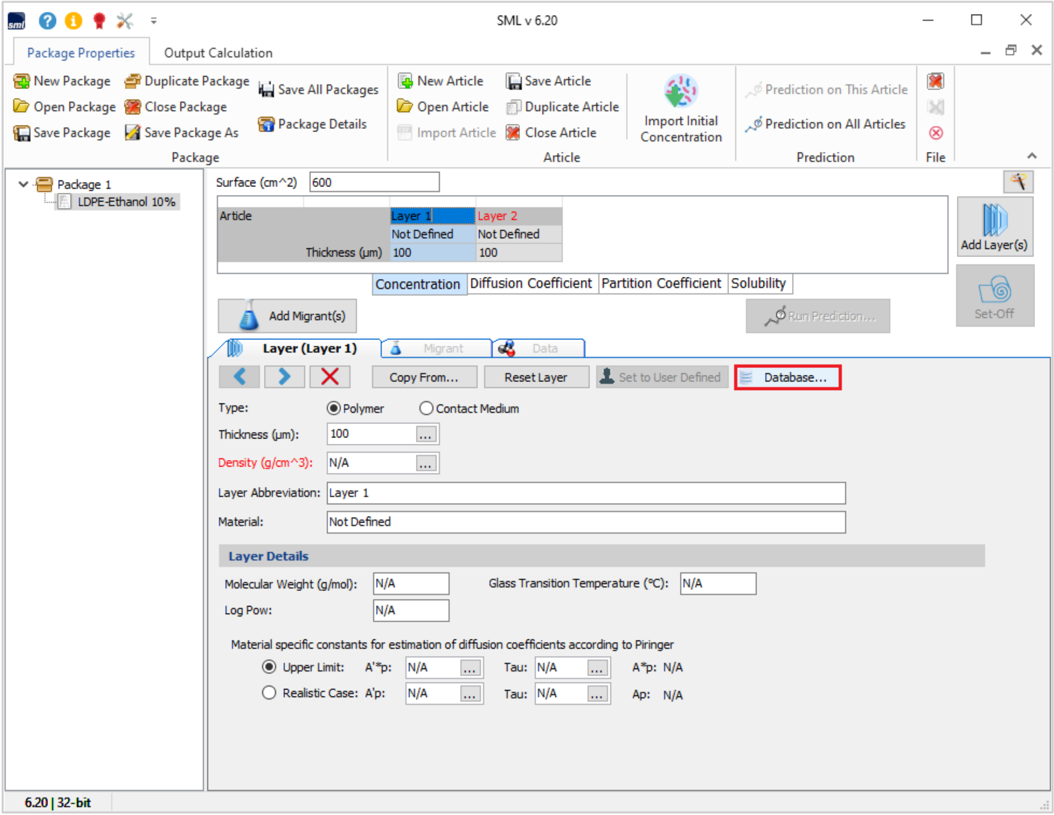


FIG. 9 - The properties of the polymer layer can be selected from the database.

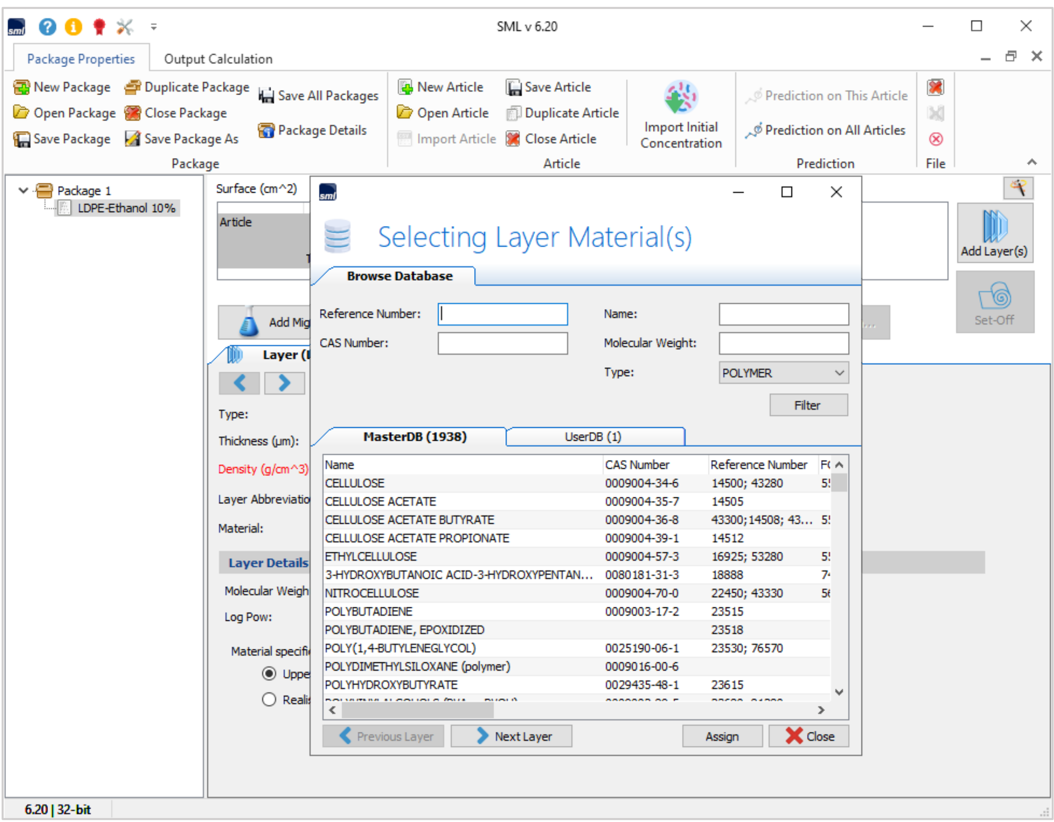


FIG. 10 – For the search of polymer properties the several options can be applied (e.g. CAS number, name, etc...).

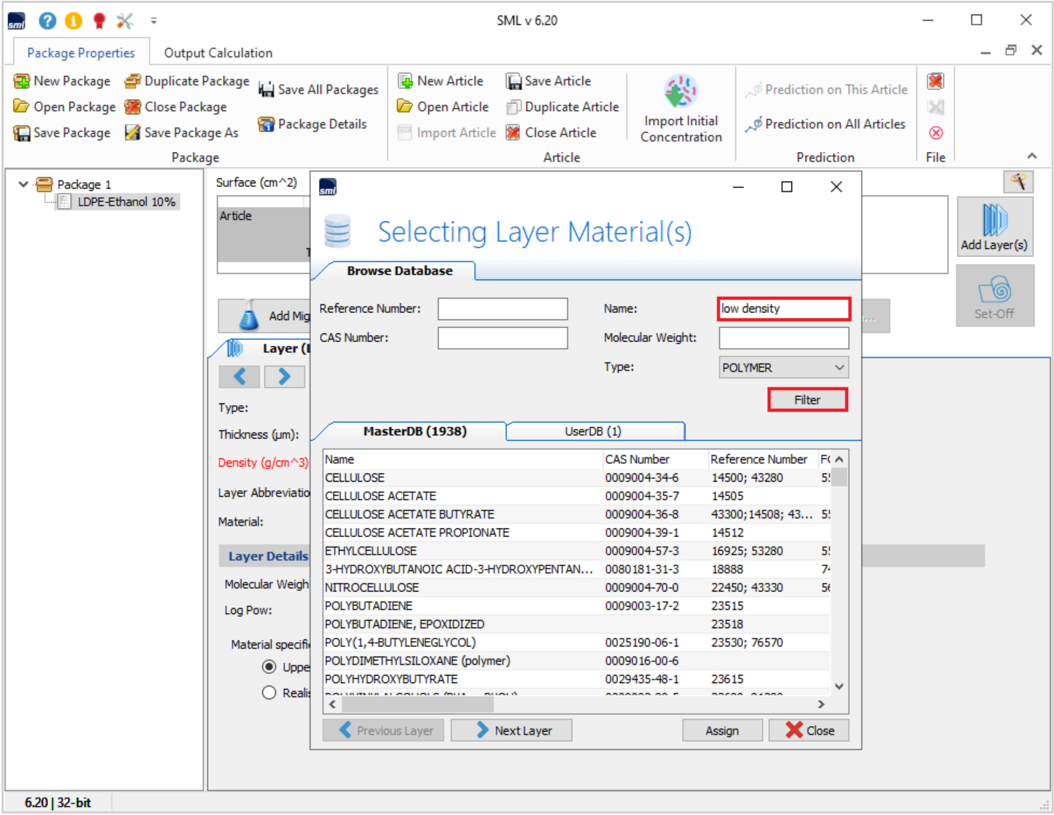


FIG. 11 - Searching the polymer by name or by specific properties (in this example, the searching key words are "low density").

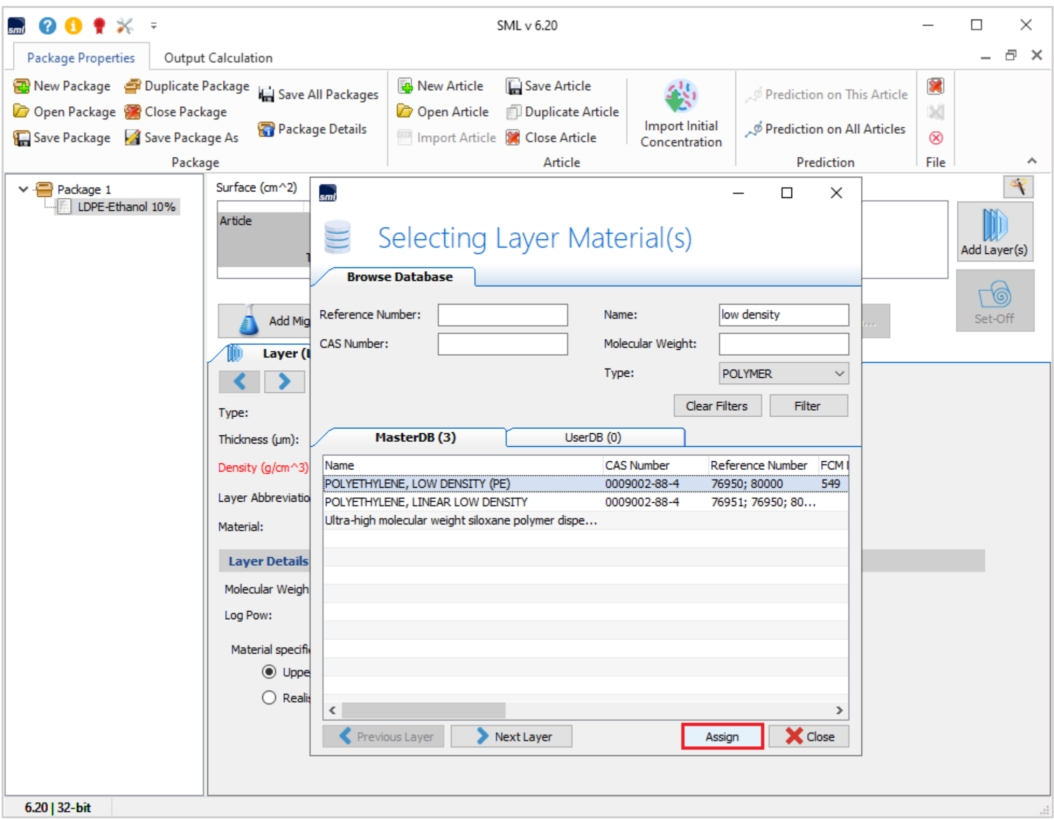


FIG. 12 - The results of the search: selection of the polymer.

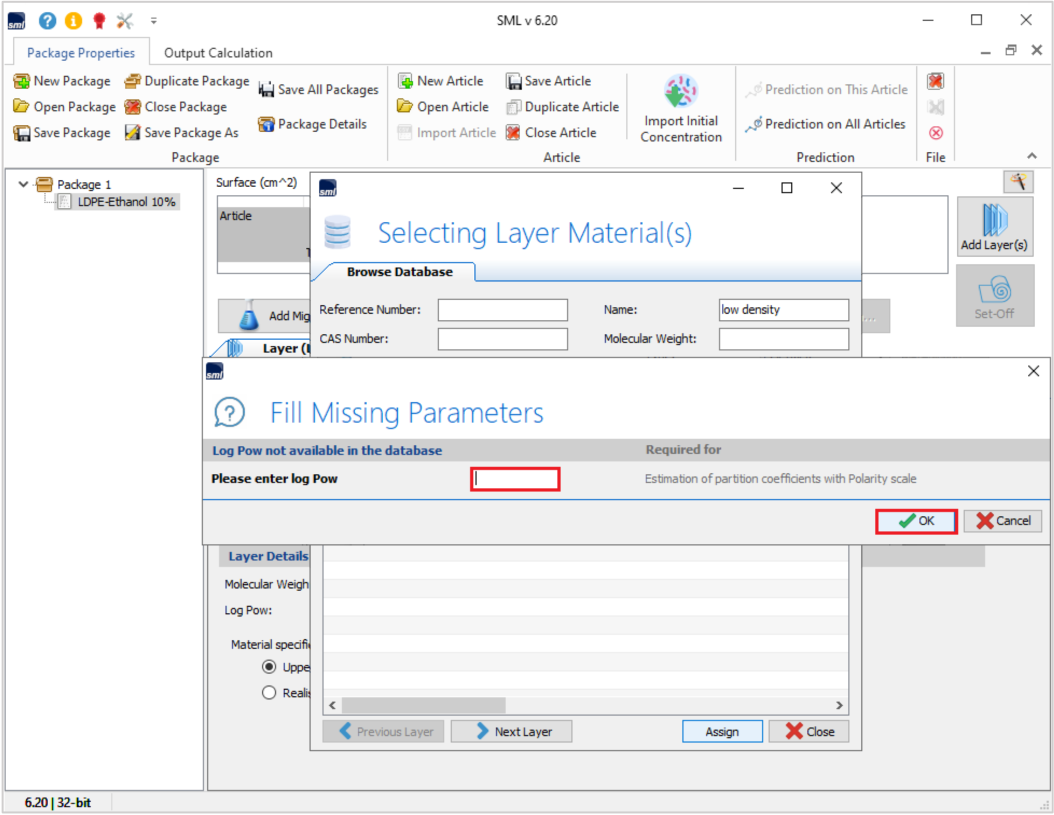


FIG. 13 - Enter missing parameters (if known). In this example the log Pow is missing.

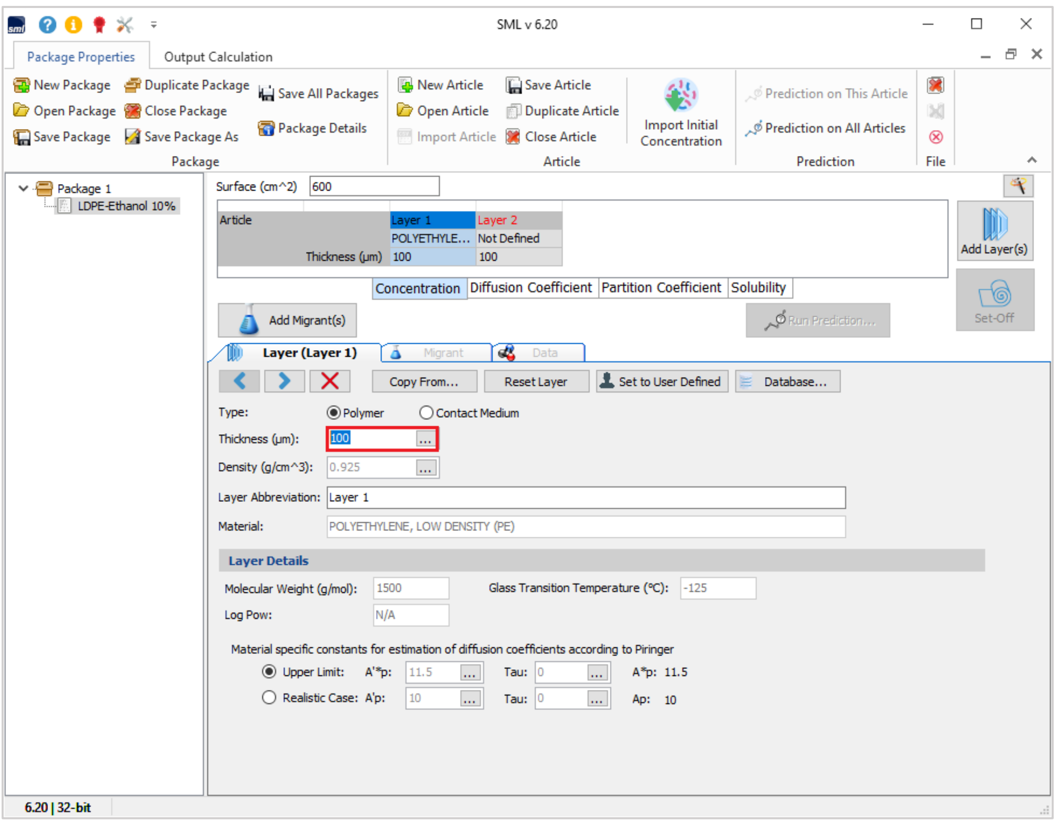


FIG. 14 - Introducing thickness of the polymer layer.

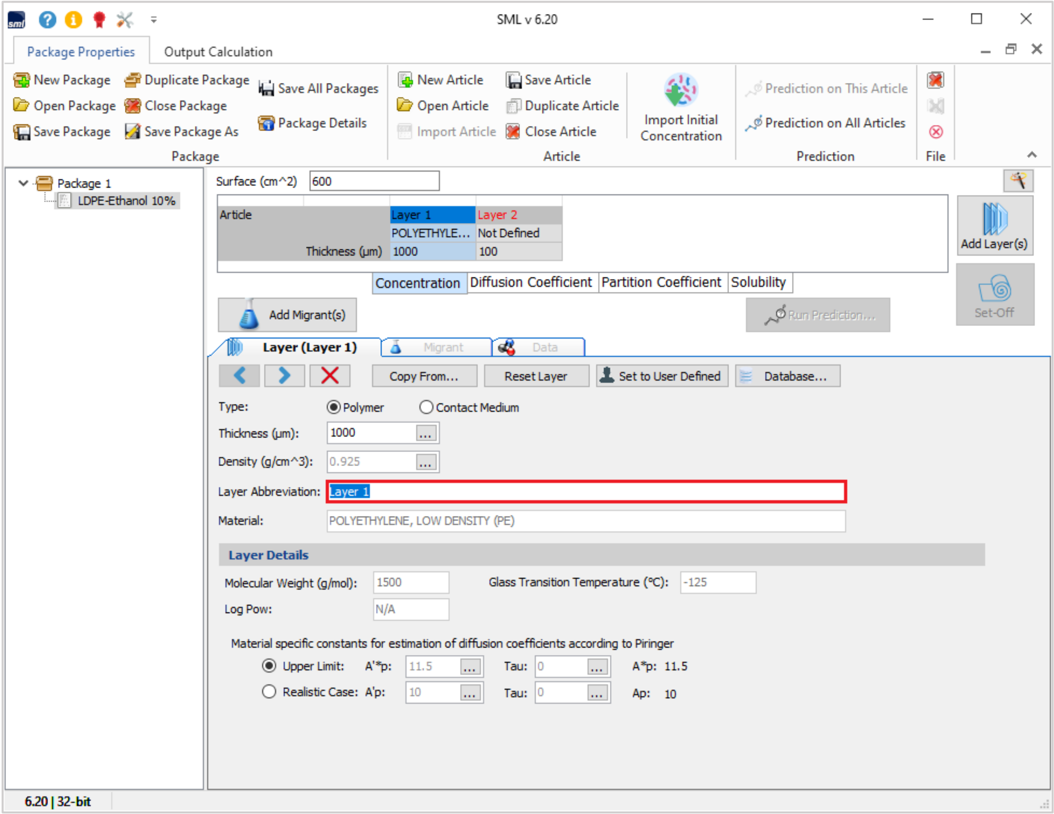


FIG. 15 – The name of the layer can be changed (if requested).

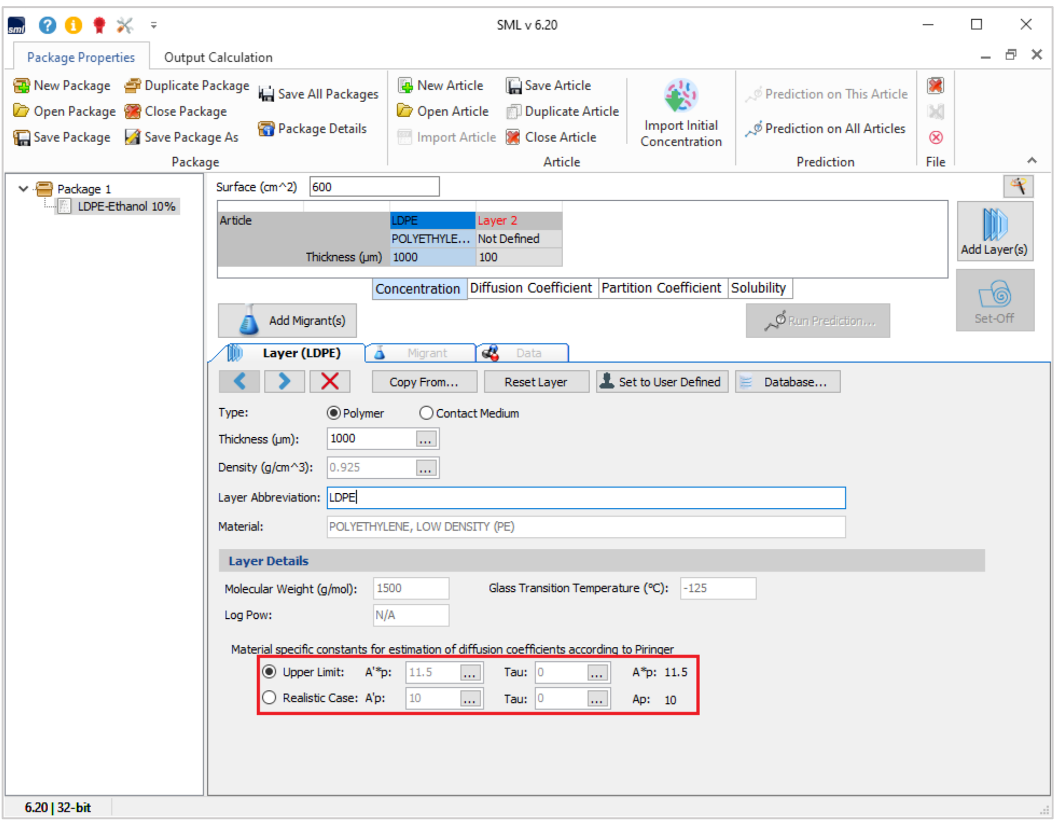


FIG. 16 - Introducing materials specific constants required for estimation of the diffusion coefficients by Piringer method with 'upper limit' or 'realistic case' calculation.

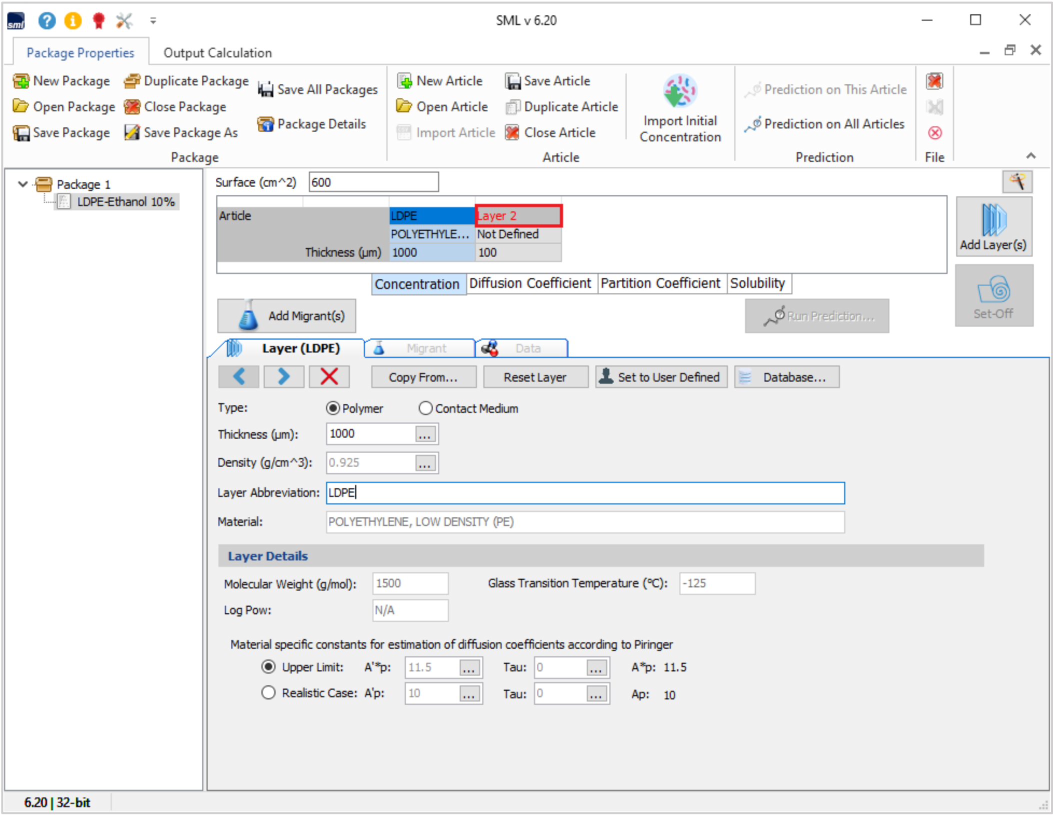


FIG. 1 - Selection of the next layer, 'layer 2'.

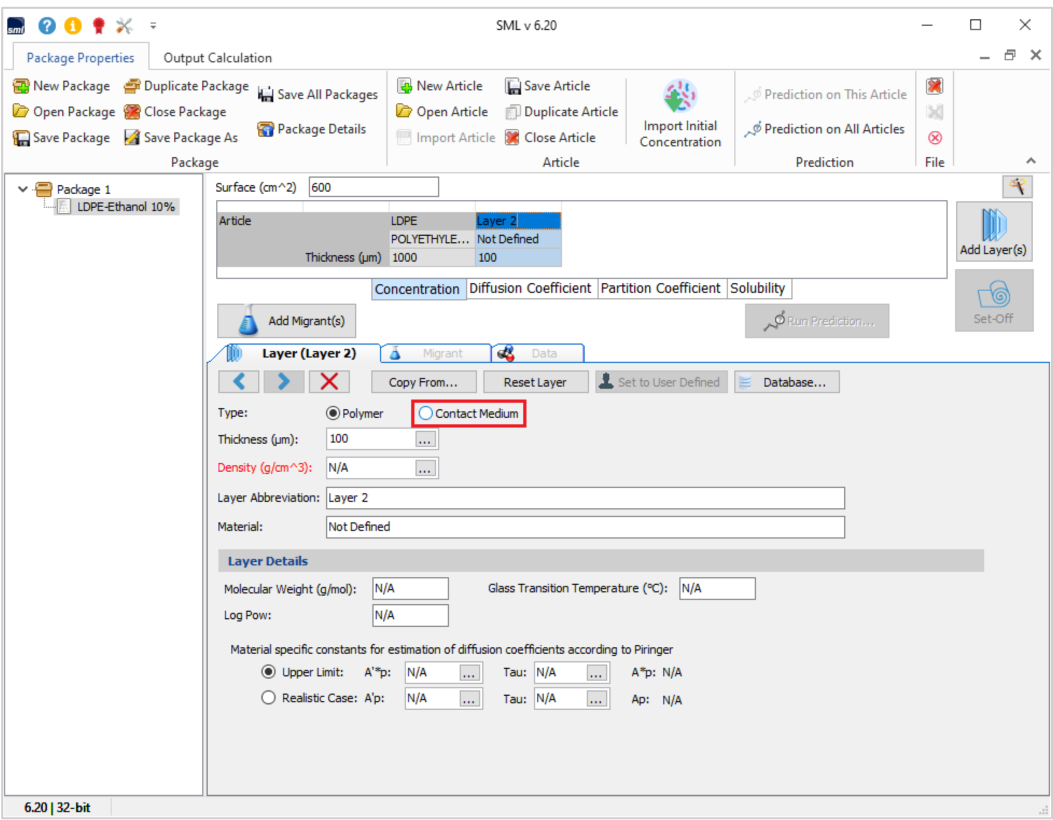


FIG. 2 – For the layer 2 the change from 'polymer' into a 'contact medium' is required.

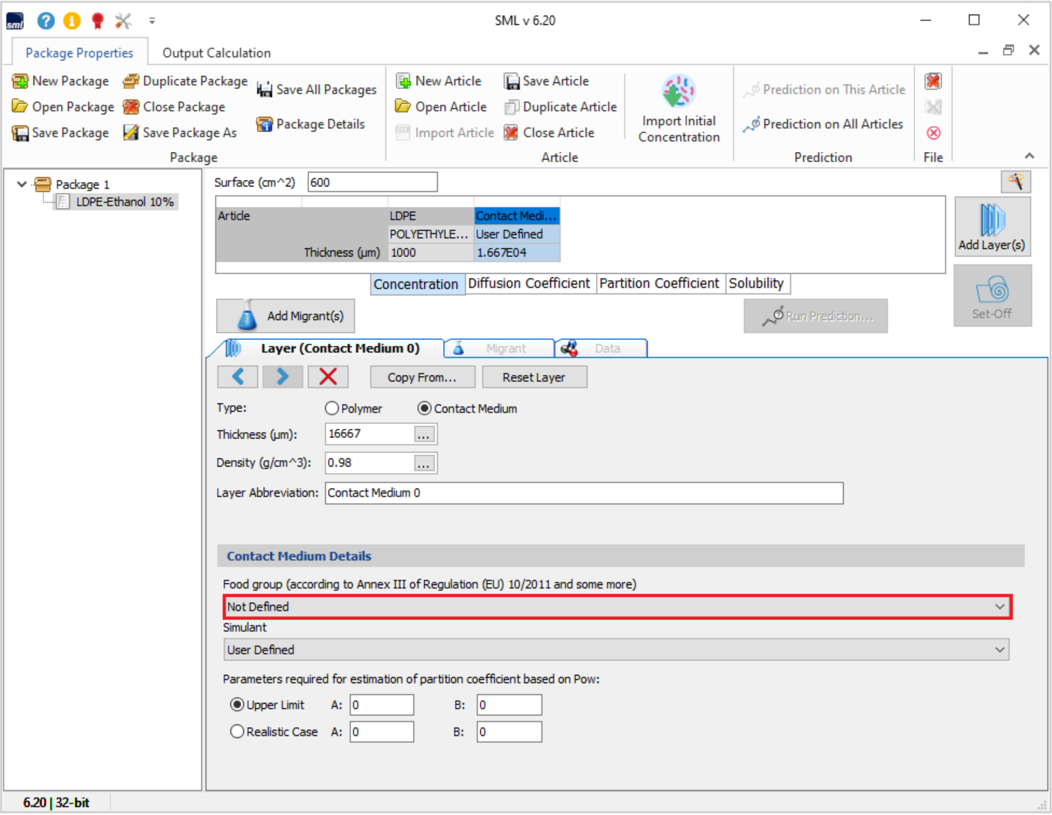


FIG. 3 - Defining the contact medium by searching in the Food Group (click on 'Not Defined' to select the food group).

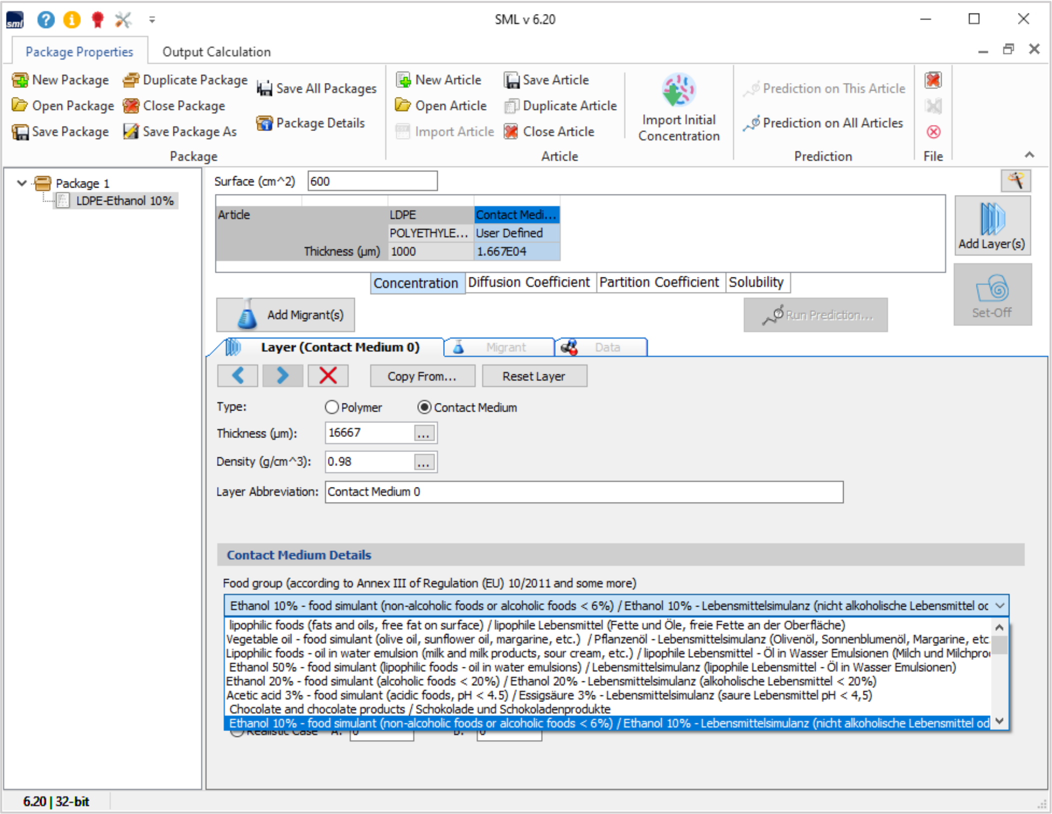


FIG. 4 - Selection of the requested food group (in English and Deutsch).

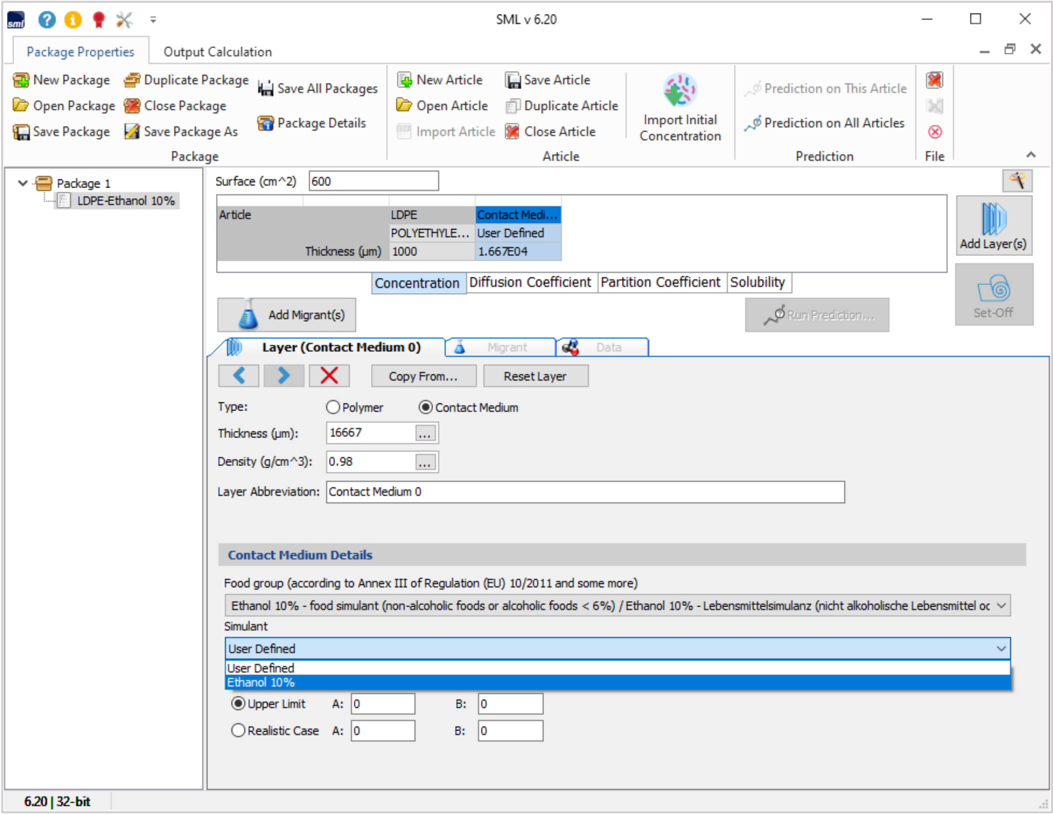


FIG. 5 - Selection of the 'Ethanol 10%' as a contact medium.

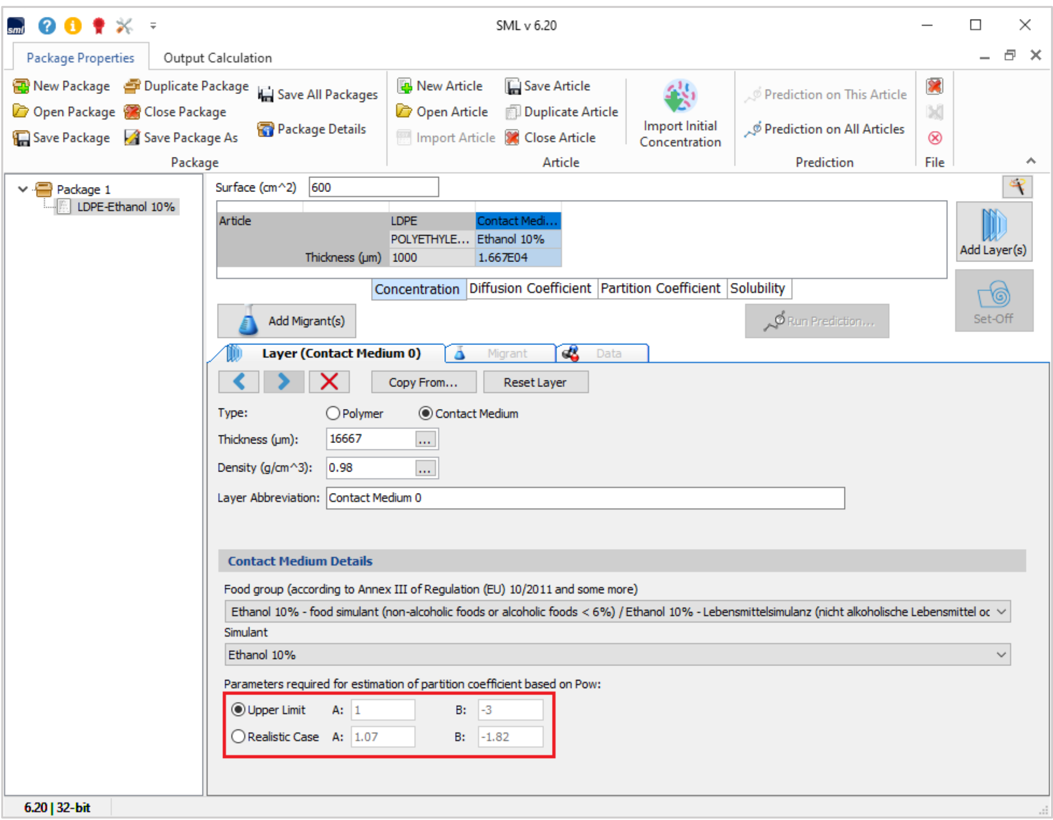


FIG. 6 - Introducing parameters required for estimation of the Octanol / Water partition coefficient by 'upper limit' or 'realistic case' method.

MIGRANTS

The migrant properties panel allows defining the properties of the currently selected migrant. When the migrant is set as user-defined, it is possible to enter its properties manually. Otherwise, if the migrant is loaded from the database, its properties are filled automatically.

The database allows browsing for known migrants (more than 20’000 chemicals: additives, monomers, photoinitiators, pigments, solvents, etc.).

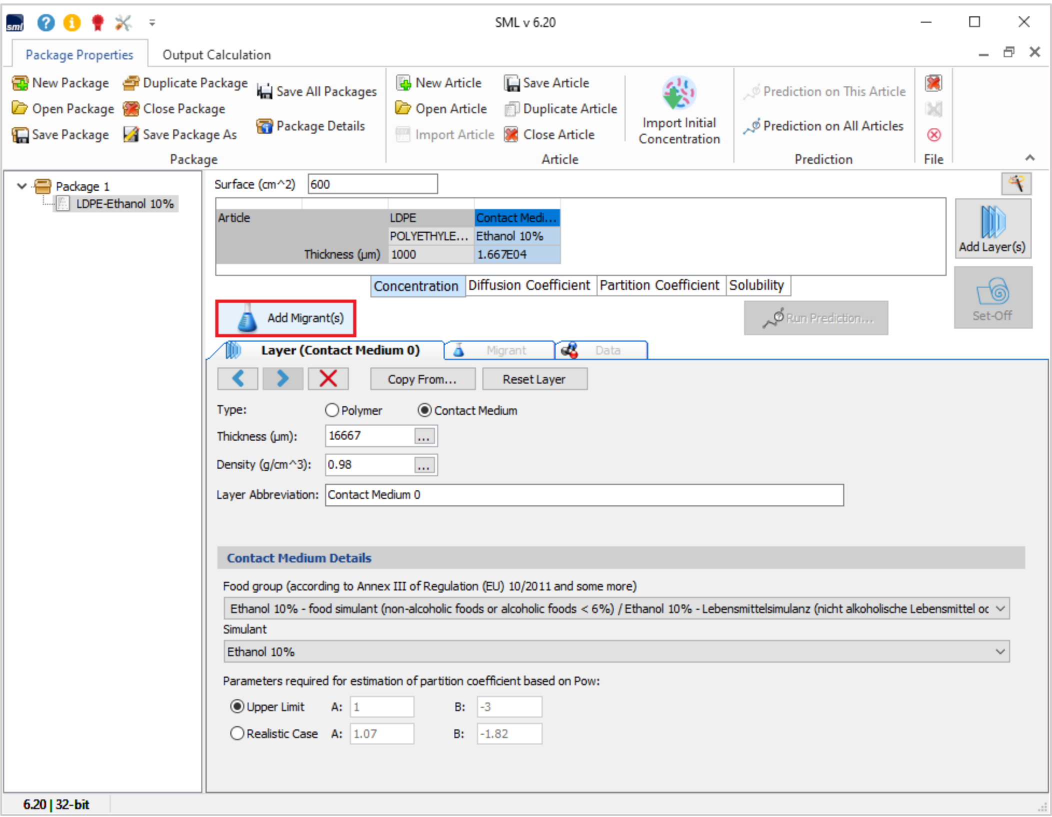


FIG. 1 - Adding migrants.

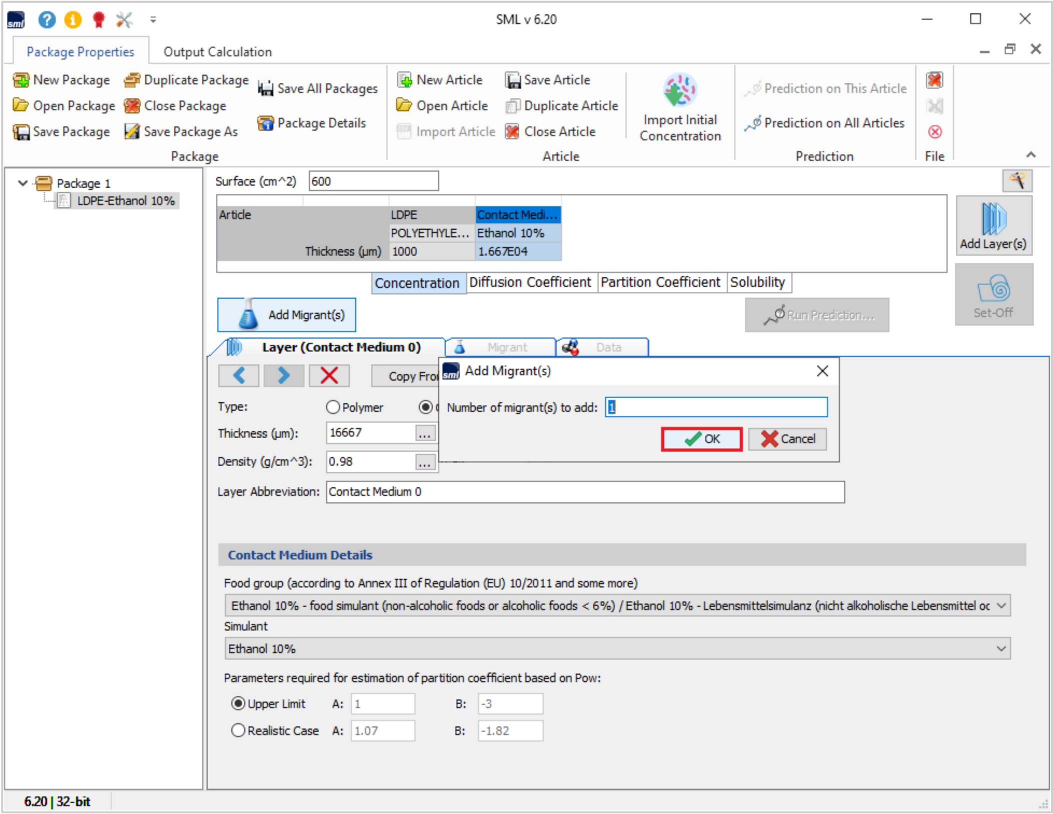


FIG. 2 - Introducing number of migrants.

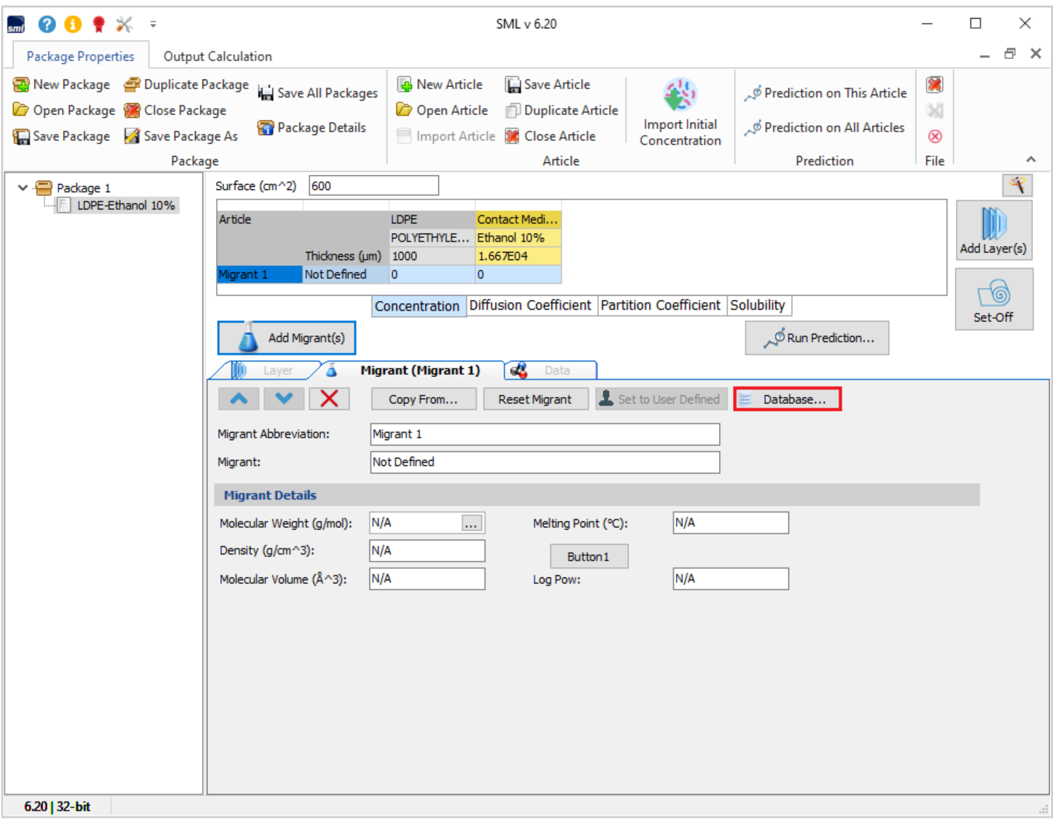


FIG. 3 - The properties of Migrants can be found in the database.

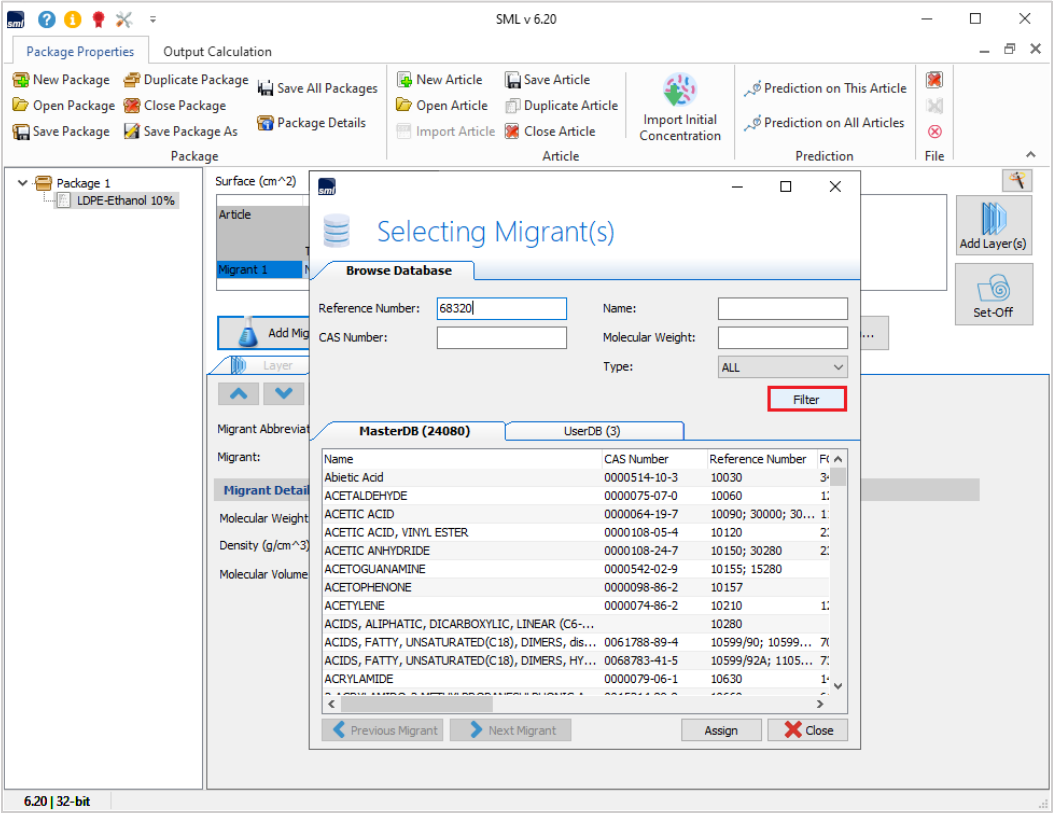


FIG. 4 - Searching for the migrant in the database by using the ‘reference number’ option.

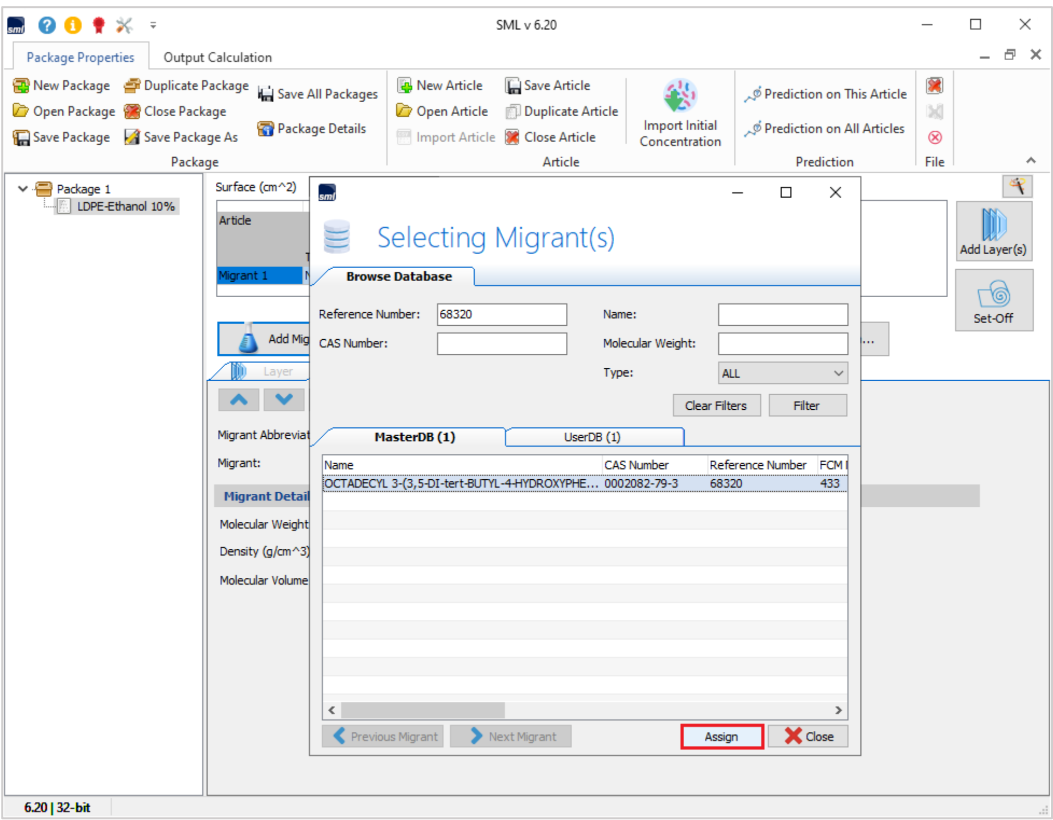


FIG. 5 - Selection of the required migrant by clicking the button “Assign”.

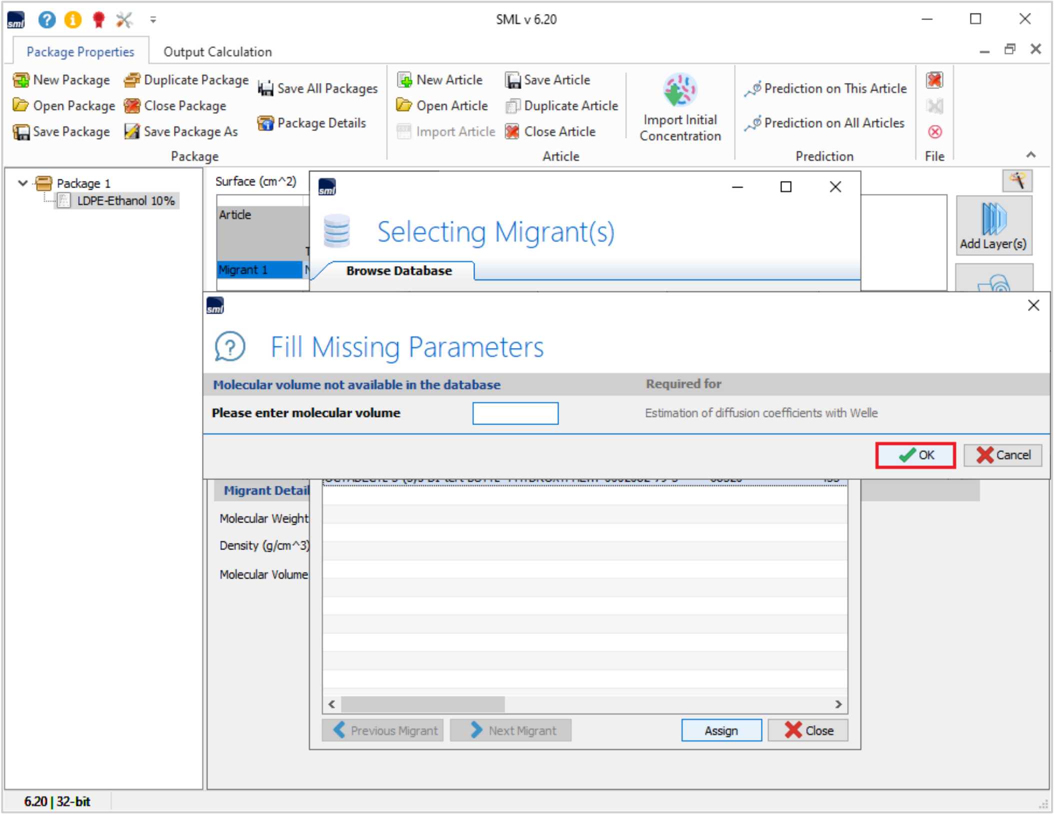


FIG. 6 - Missing parameters, here the Molecular Volume, can be added (if known).

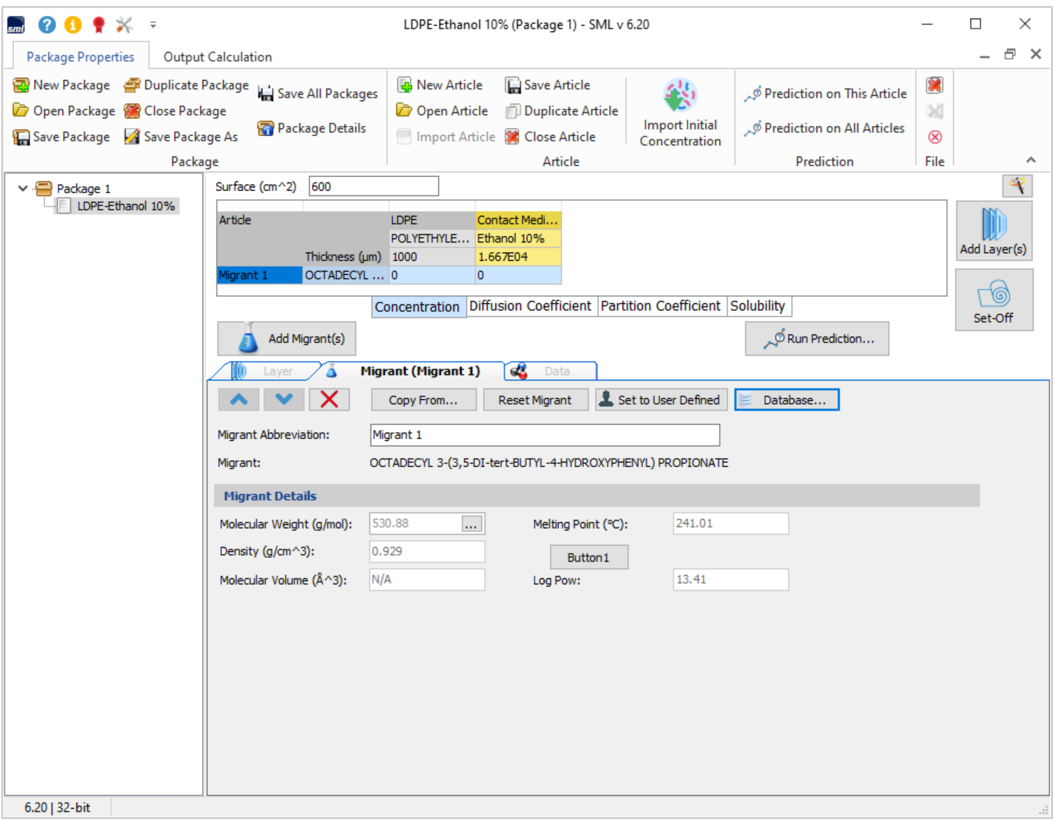


FIG. 7 - Layers of the article and migrant are defined.

MIGRANTS PROPERTIES (CONCENTRATION, DIFFUSION AND PARTITION COEFFICIENT

For the prediction of the migration process, it is necessary to introduce the key parameters of the migrant:

- The concentration
- The diffusion coefficient
- The partition coefficient

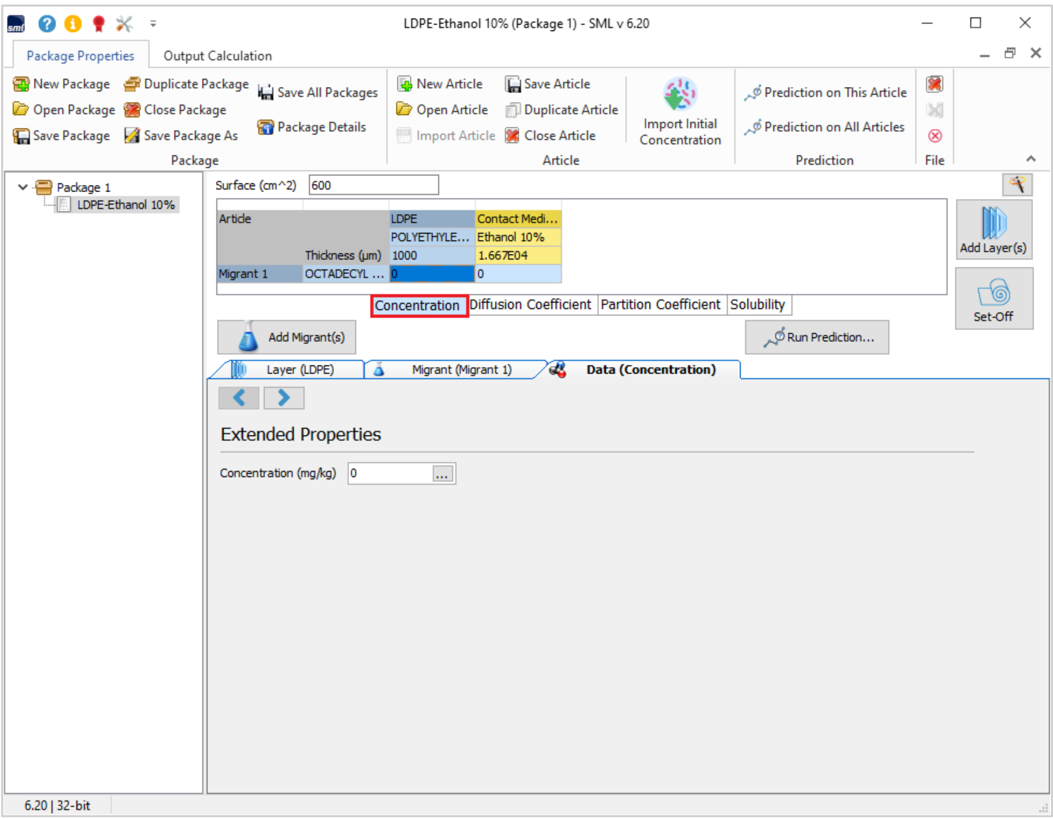


FIG. 1 - Defining the migrant concentration.

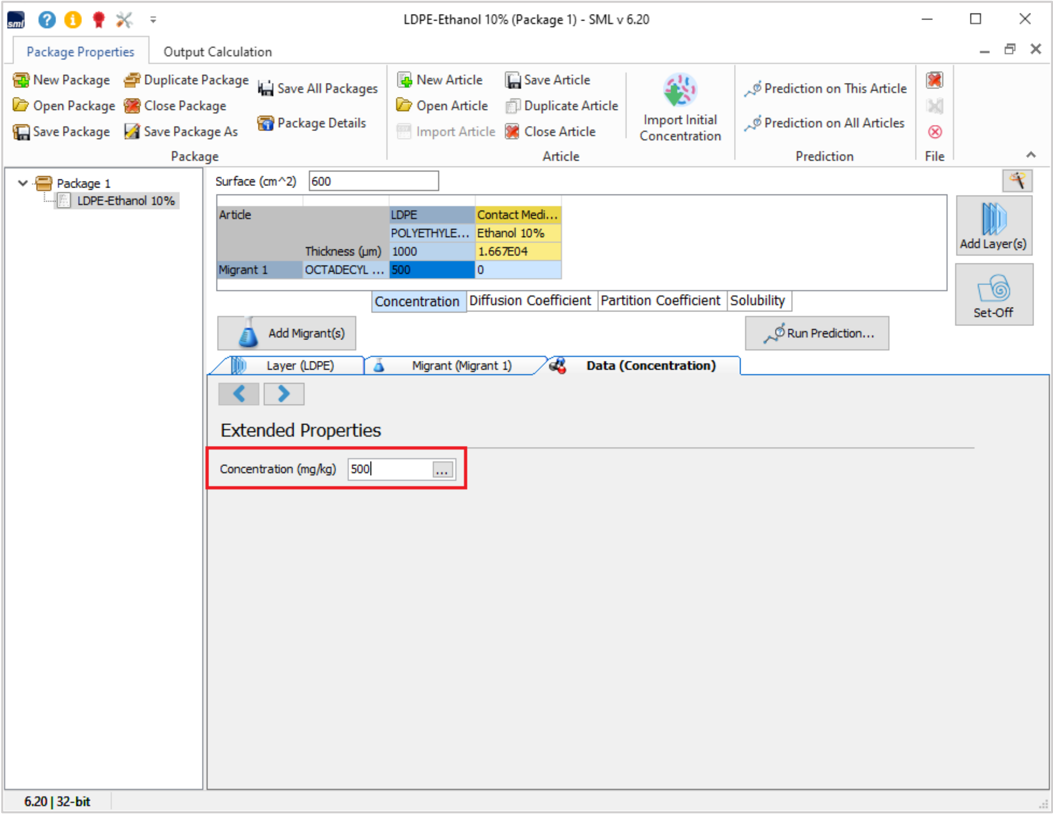


FIG. 2 - Introducing concentration of migrant in mg/kg (ppm).

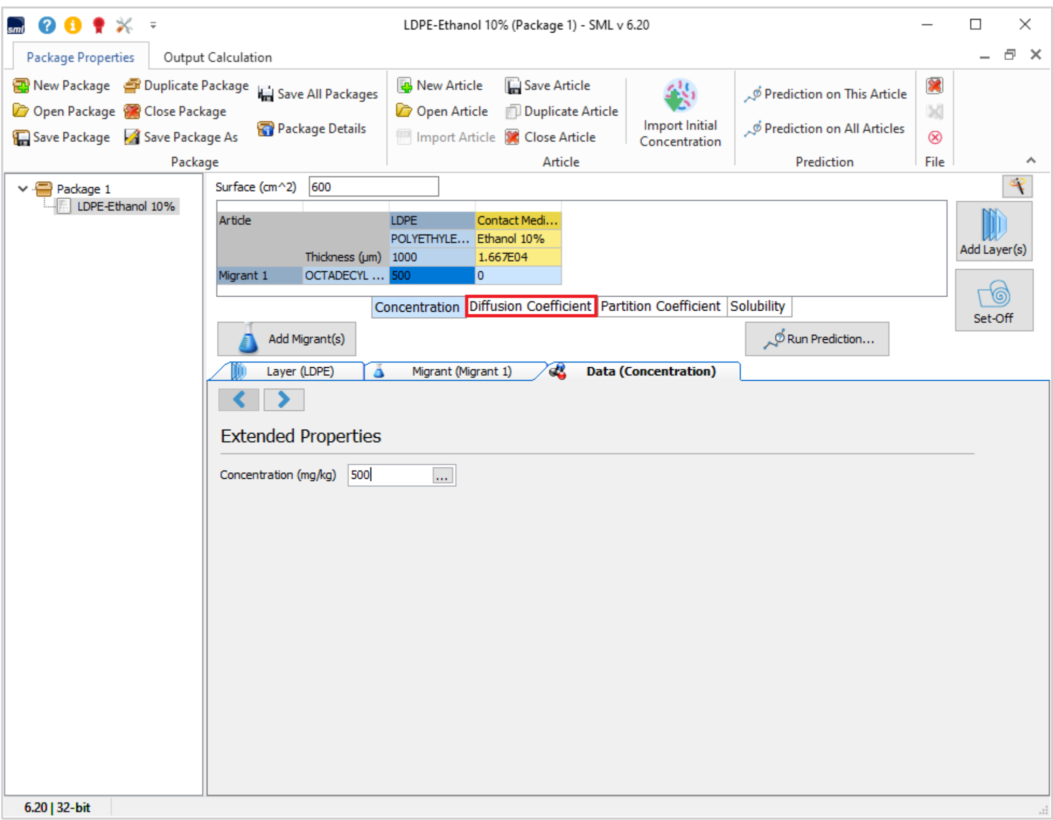


FIG. 3 - Selection of diffusion coefficient.

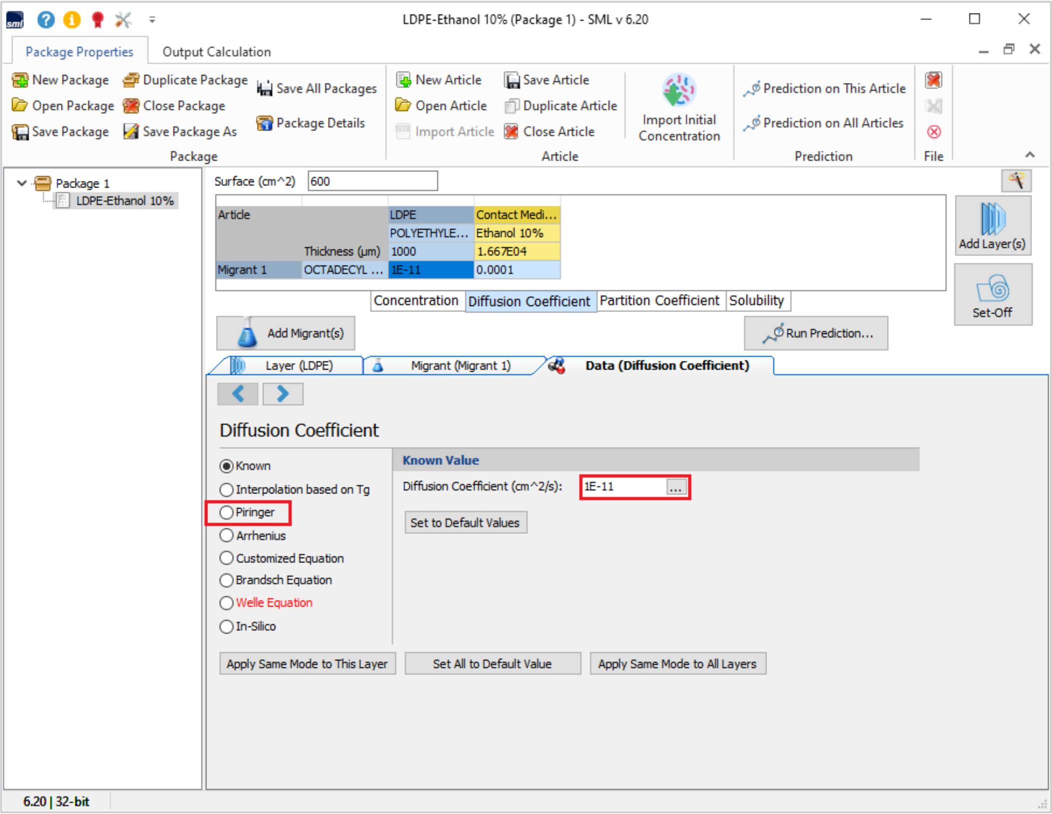


FIG. 4 - Introducing diffusion coefficient (if known, here 1e-11 is a default value) or selection of an estimation method (e.g. Piringer). In this example the Welle equation is marked in red because its use is impossible due to the lack of parameters required in this method.

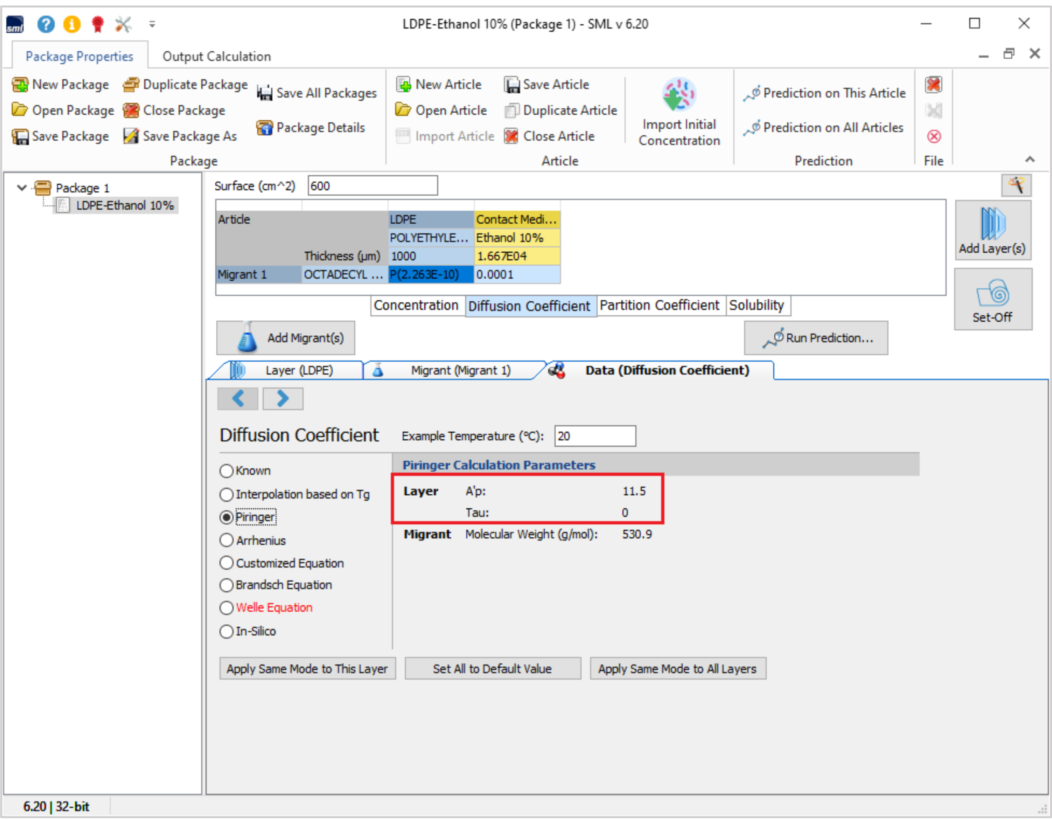


FIG. 5 - Introducing of calculation parameters (Ap and Tau) required for evaluation of Diffusion Coefficient based on Piringer method.

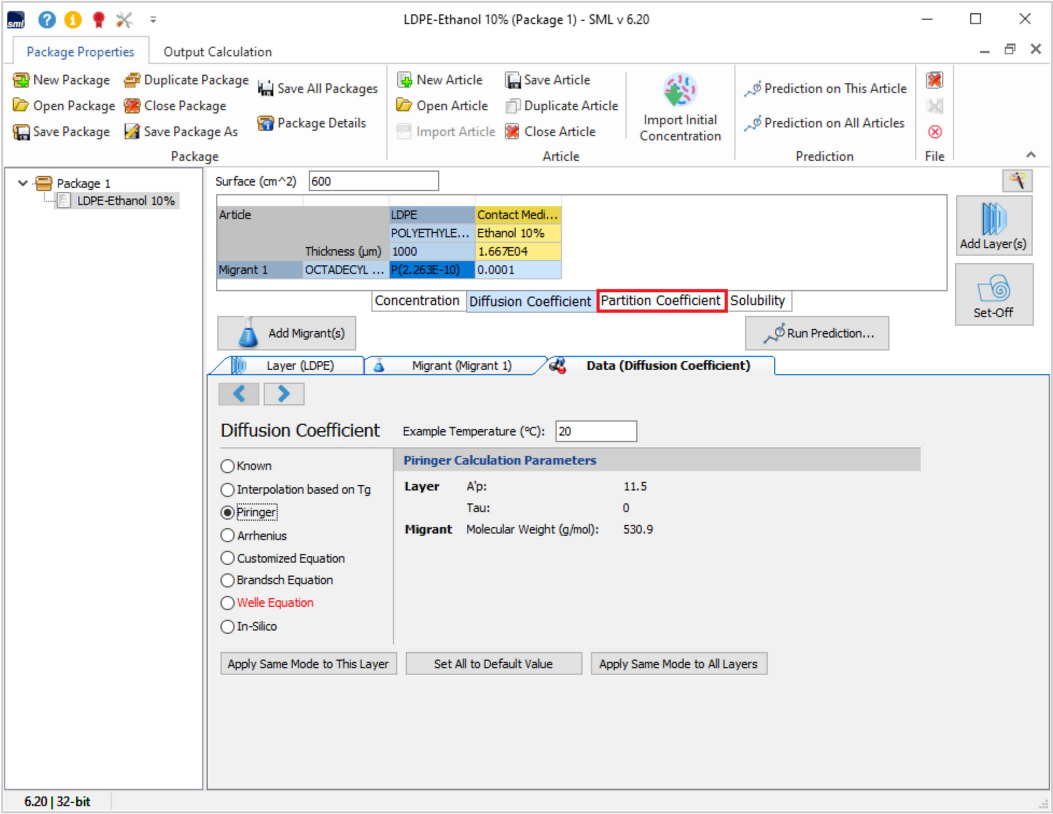


FIG. 6 - Selection of partition coefficient.

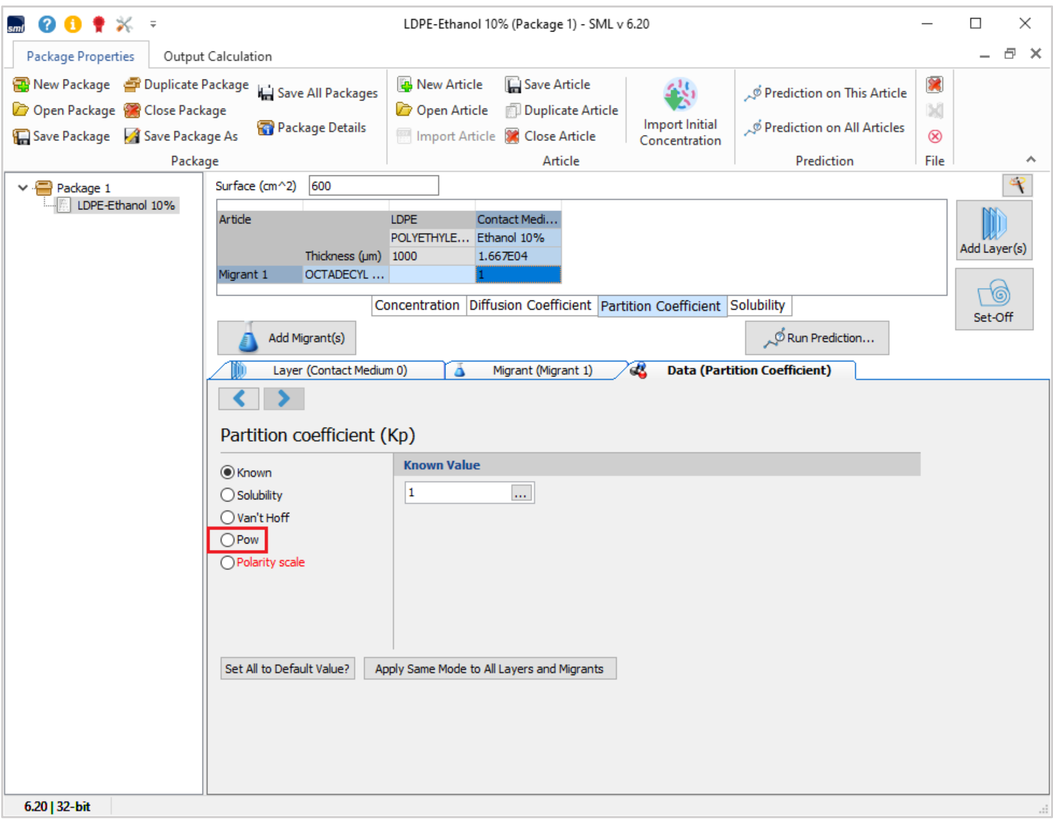


FIG. 7 - Introducing of partition coefficient (if known) or selection of an estimation method (e.g. Octanol /Water partition coefficient). In this example the Polarity Scale is marked in red and is not available because of missing polarity scale parameters. Generally, two arbitrary selected partition coefficients according to the JRC guideline are used for upper limit calculations: kpF = 1 if the migrant is soluble in the food contact material/ simulant and kpF = 1000 if the migrant is not soluble in the food contact material/ simulant. The 'POW' method uses the relationship between log POW (derived from the polarity of the migrant) and log kpF and provides a more precise partition coefficient.

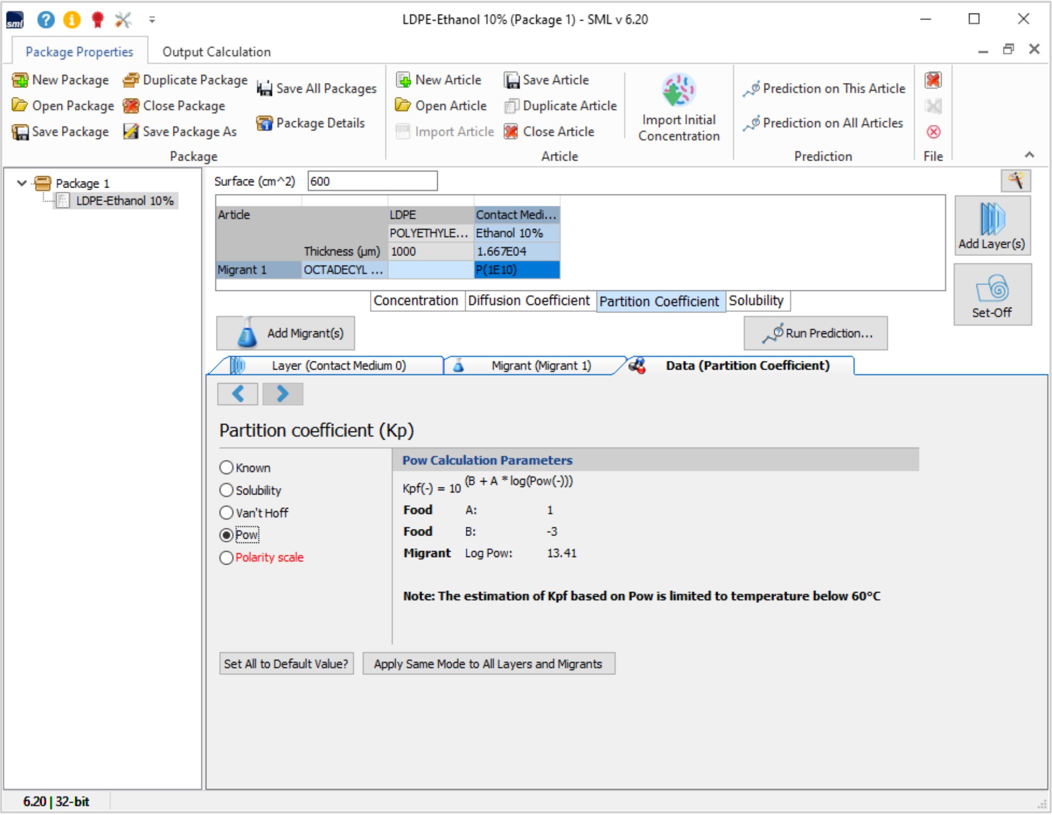


FIG. 8 - Partition coefficient based on Octanol/Water method.

When all properties of an article are introduced, it is possible to proceed with prediction calculations by clicking on the “Run Prediction” button.

The predictions of the migration can be performed for different temperature profiles:

- Isothermal
- Non-Isothermal
- Stepwise
- Modulated
- Shock
- Worldwide
- STANAG
- Customized

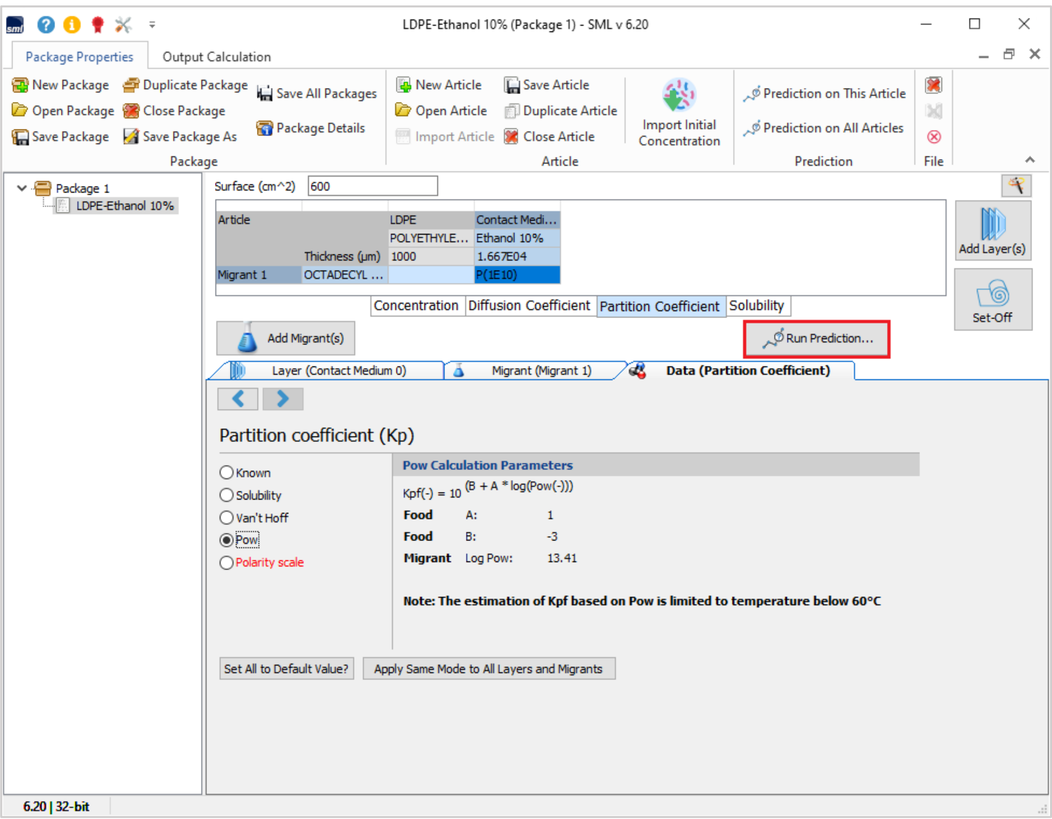


FIG. 1 - Prediction of Migration.

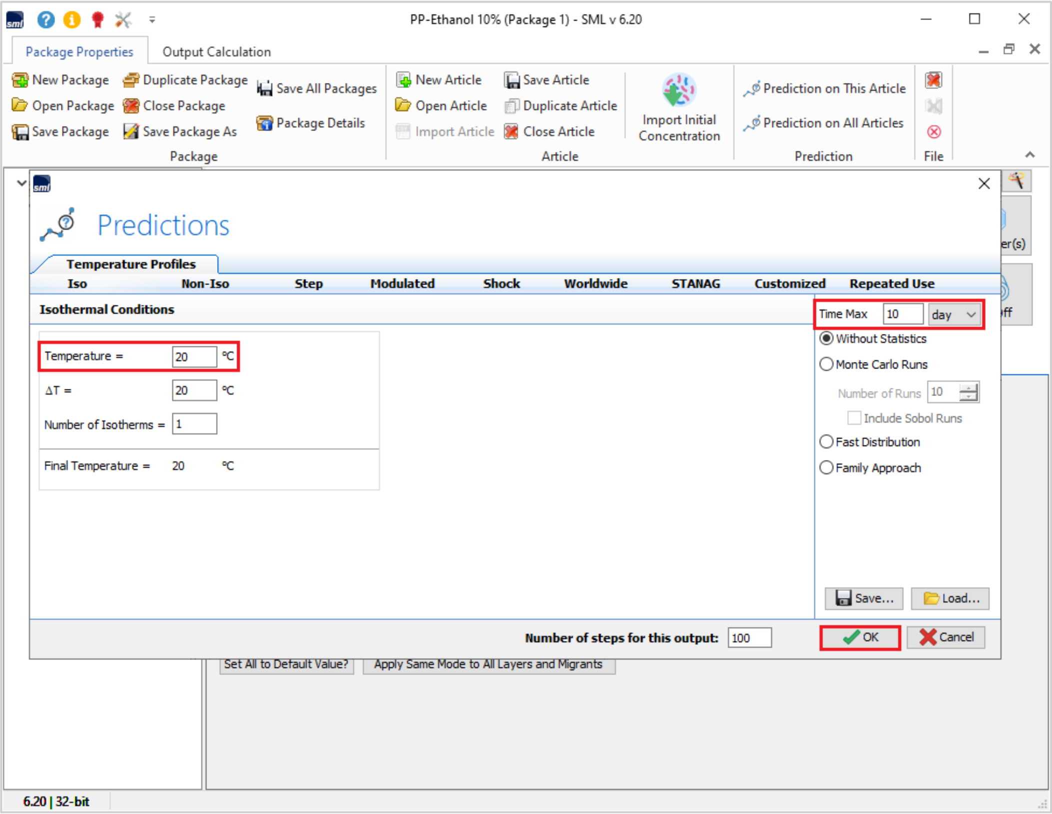


FIG. 2 - Prediction of Migration occurring under isothermal conditions (during 10 days at 20°C).

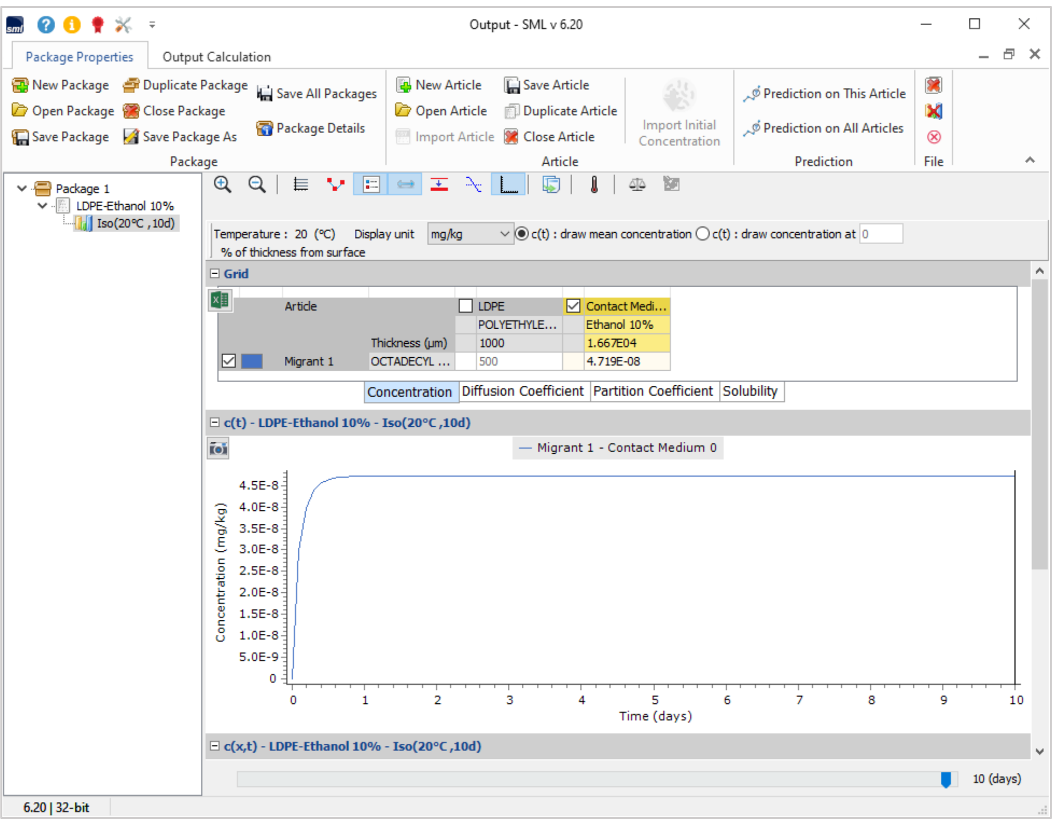
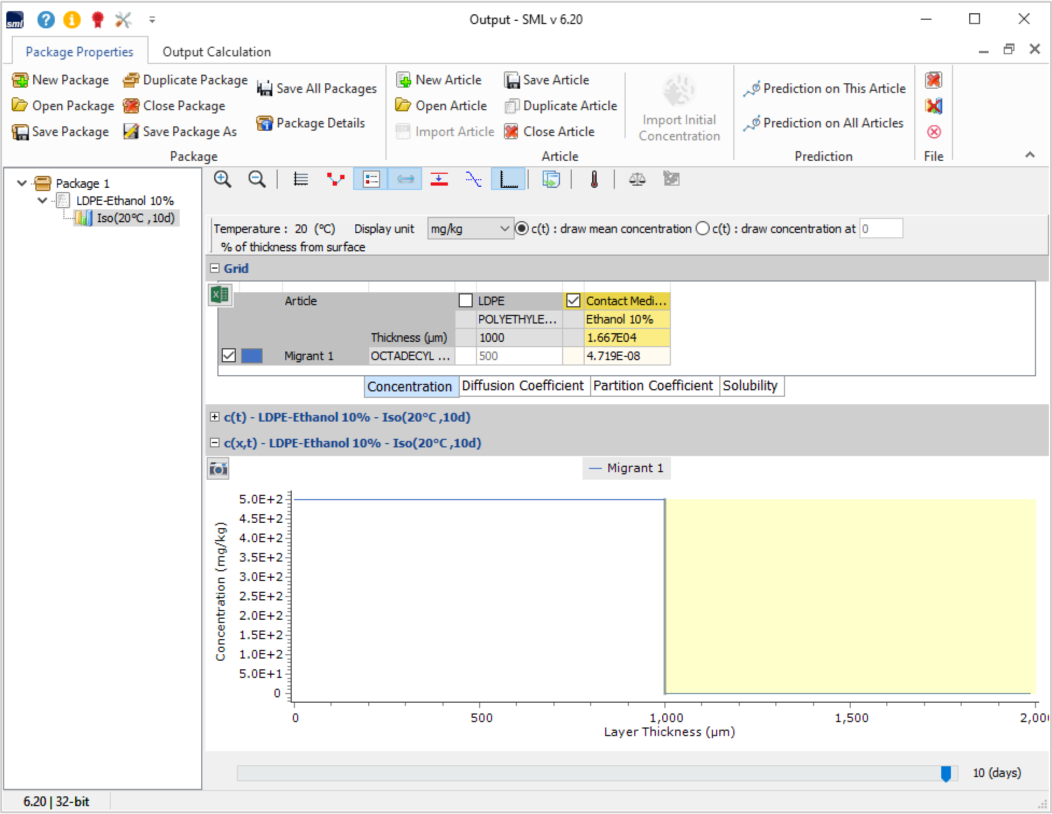
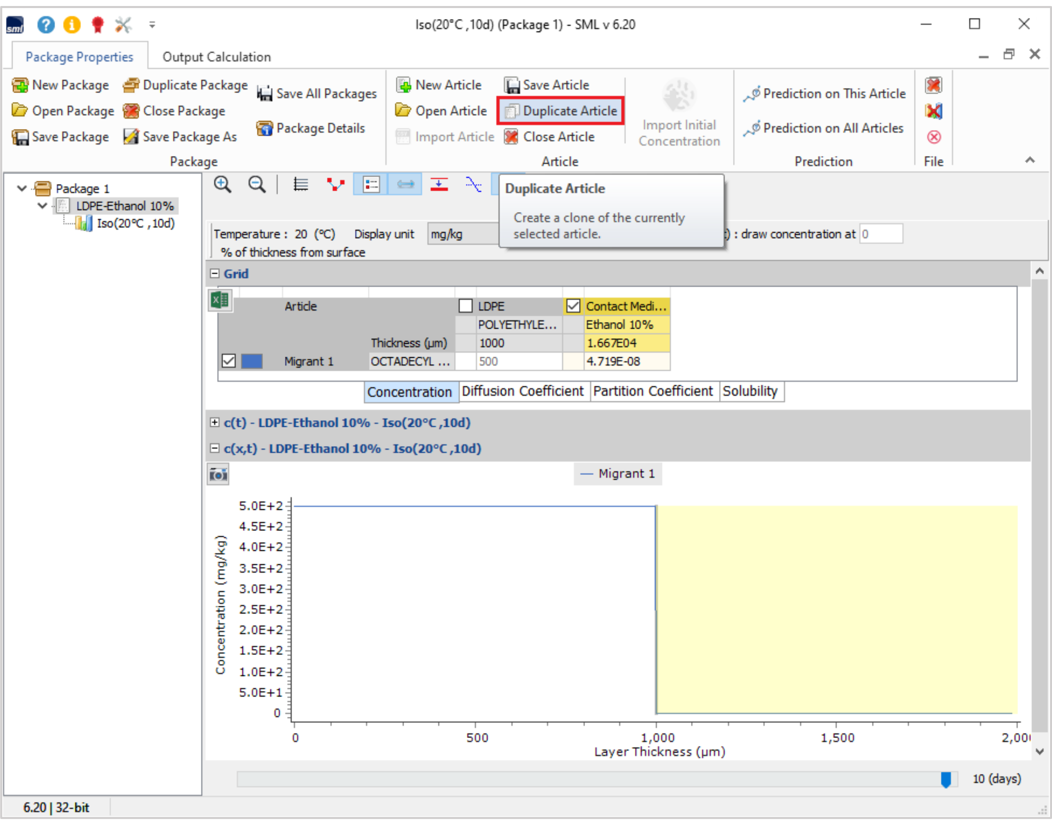


FIG. 3 - Concentration profile of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) in the contact medium over time, no migration of migrant to food simulant 'Ethanol 10%' is found.



Article	LDPE	Contact Medi...
	POLYETHYLE...	Ethanol 10%
Thickness (µm)	1000	1.667E04
Migrant 1 OCTADECYL ...	500	4.719E-08

FIG. 4 - Concentration profile of migrant over layer thickness and time (no migration to food simulant).



Article	LDPE	Contact Medi...
	POLYETHYLE...	Ethanol 10%
Thickness (µm)	1000	1.667E04
Migrant 1 OCTADECYL ...	500	4.719E-08

FIG. 5 - Apply the option 'Duplicate Article' to modify the article properties in a new simulation.

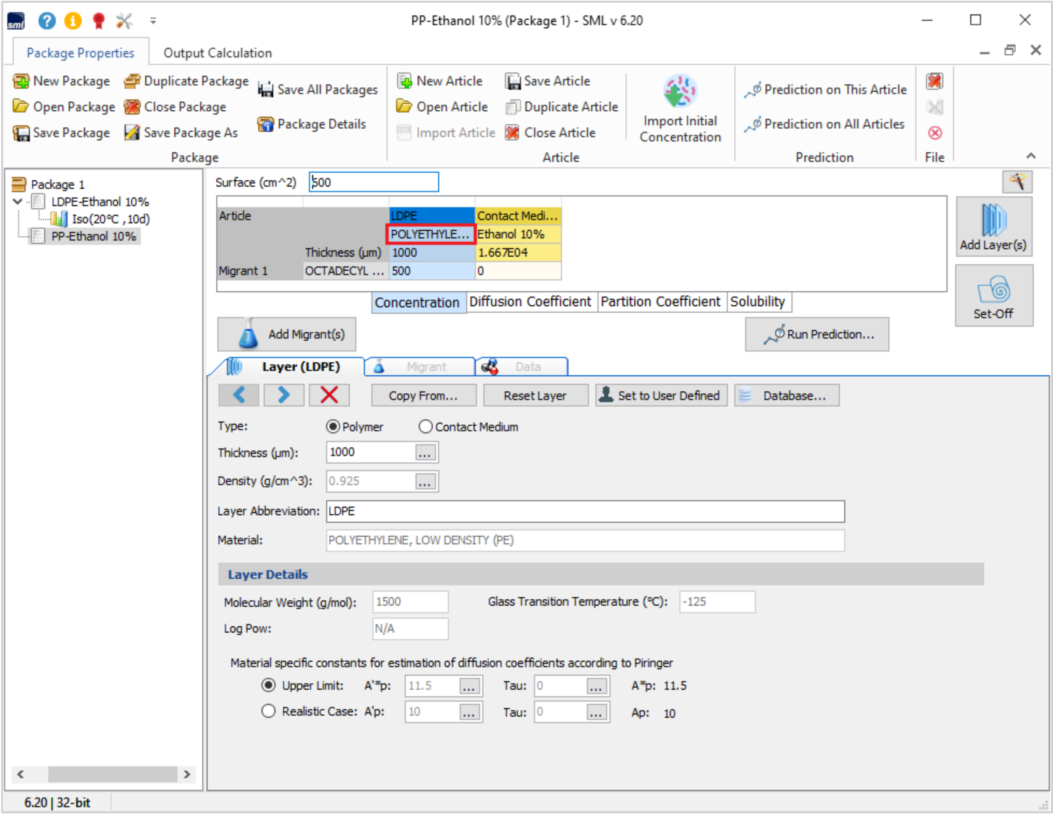


FIG. 6 - Selection of the polymer layer.

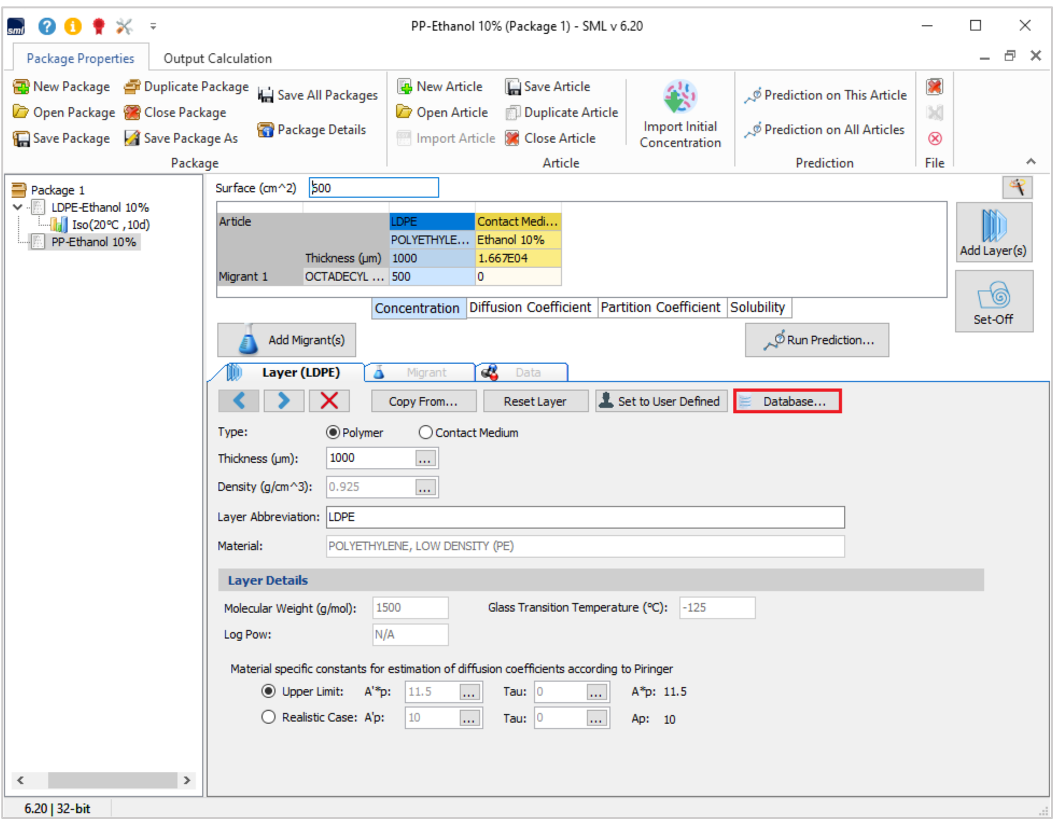


FIG. 7 - Selecting a new polymer from the database.

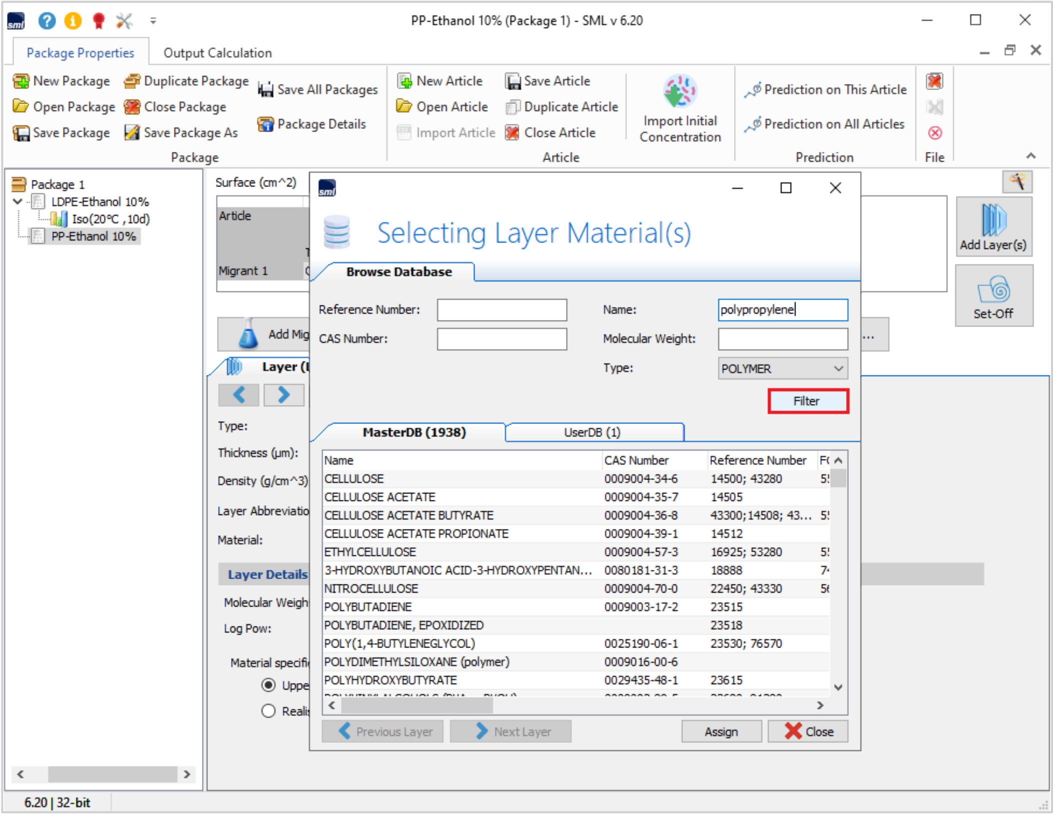


FIG. 8 - Searching for 'polypropylene'.

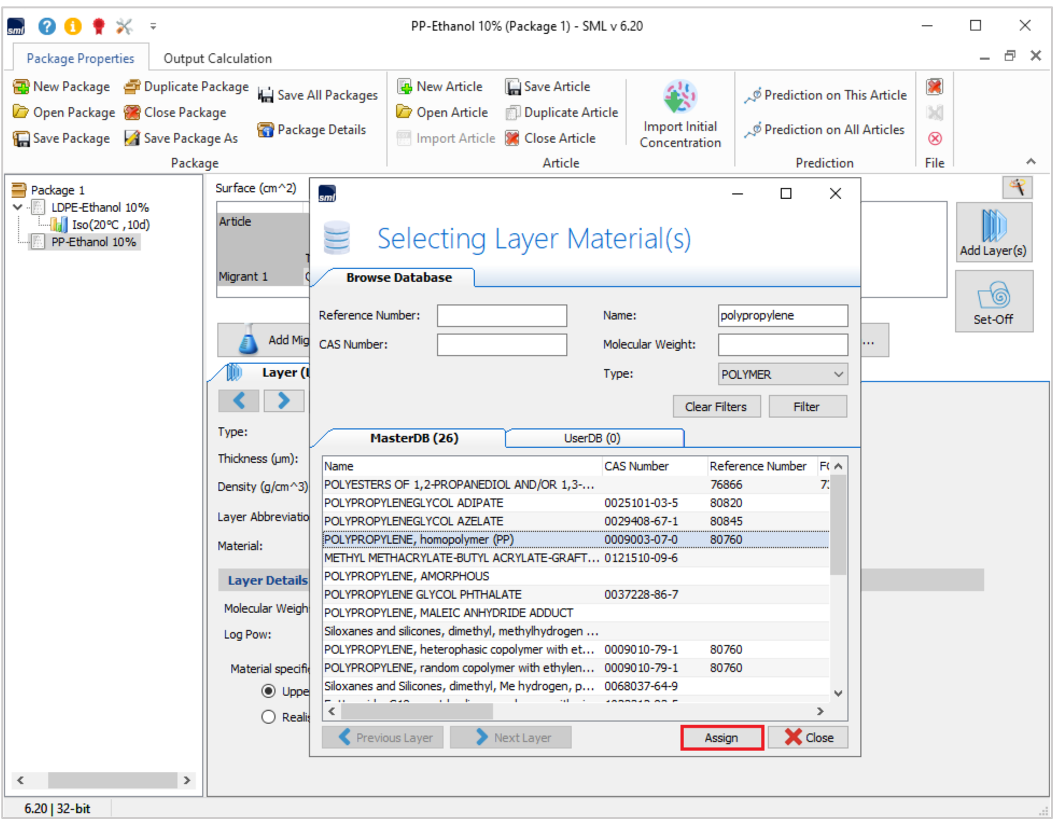


FIG. 9 - Selection of 'polypropylene'.

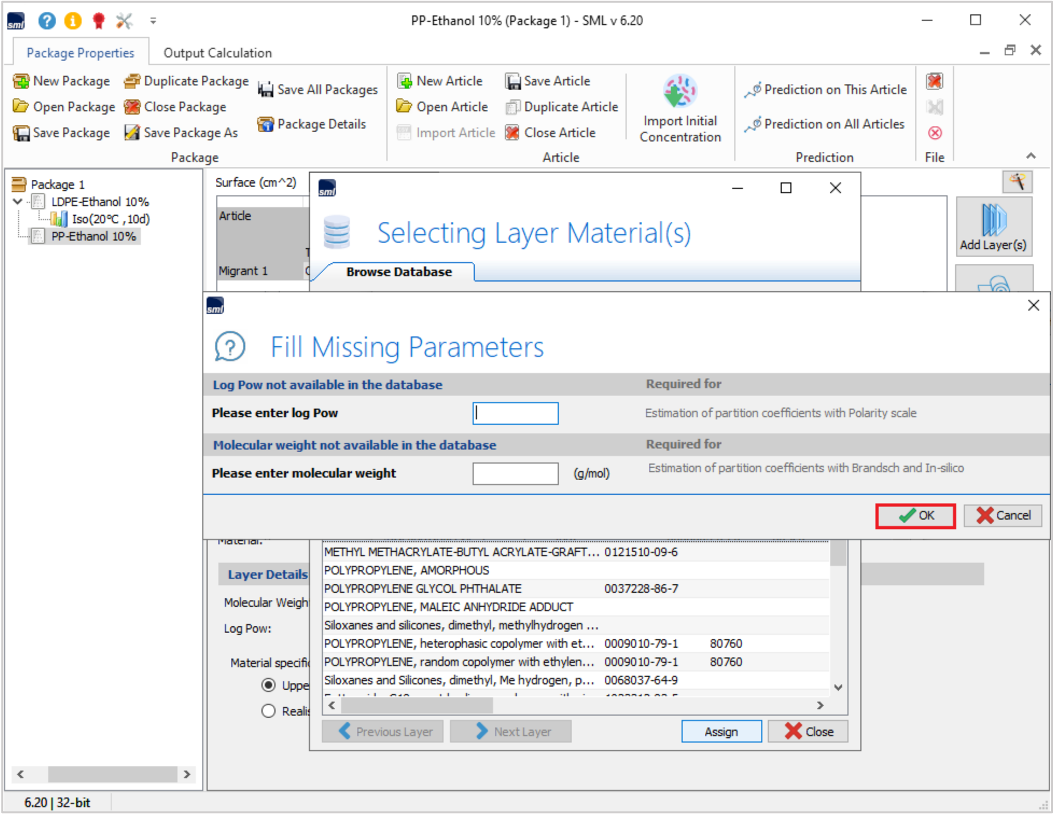


FIG. 10 - Adding of missing parameters (if known).

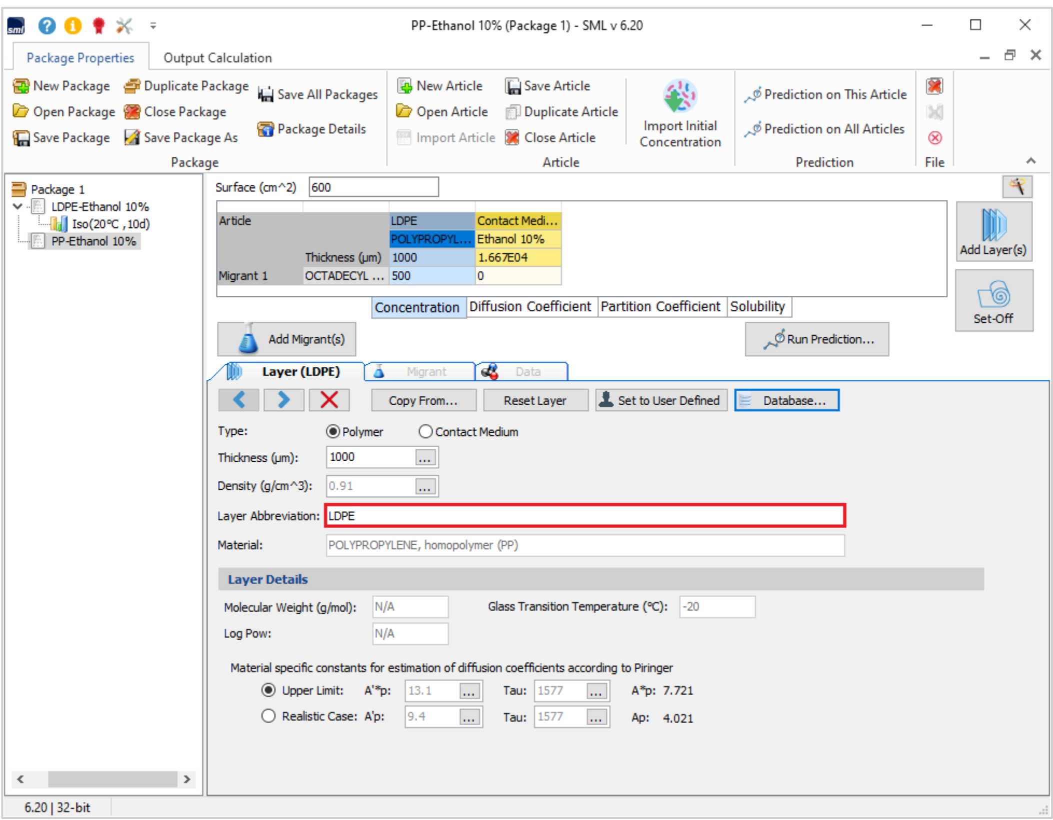


FIG. 11 - Layer abbreviation should be accordingly corrected in case of changing the polymer.

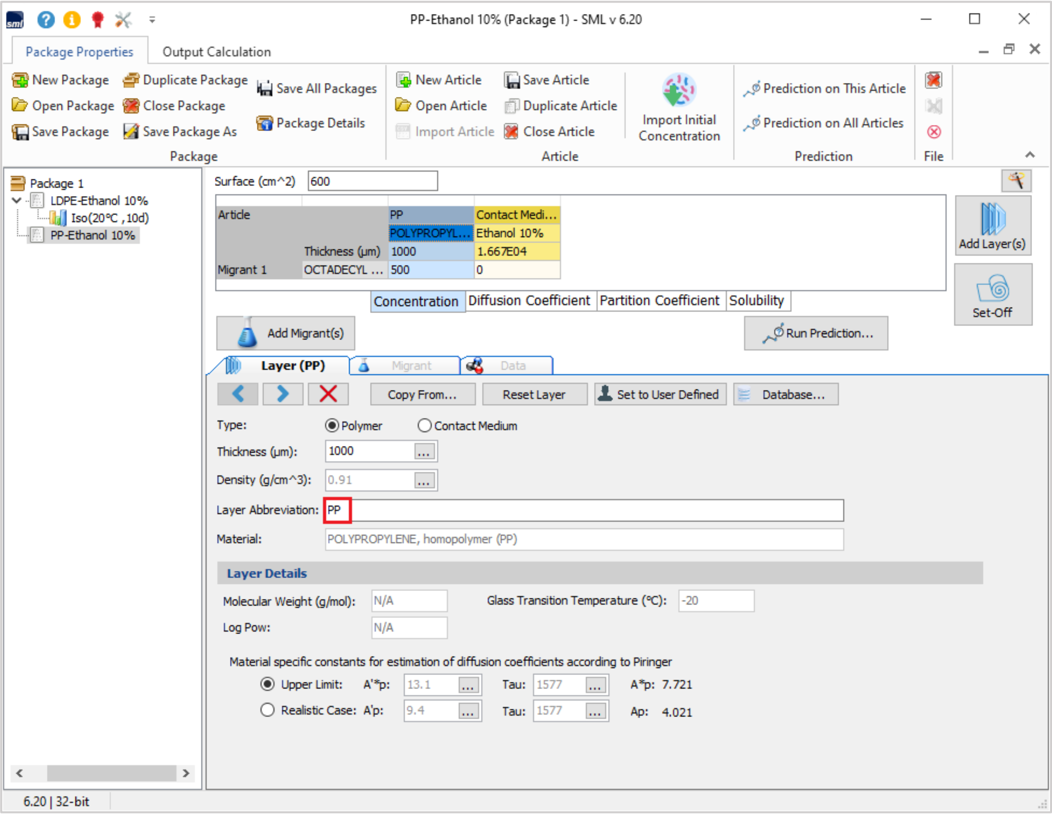


FIG. 12 - Layer abbreviation changed to 'PP'.

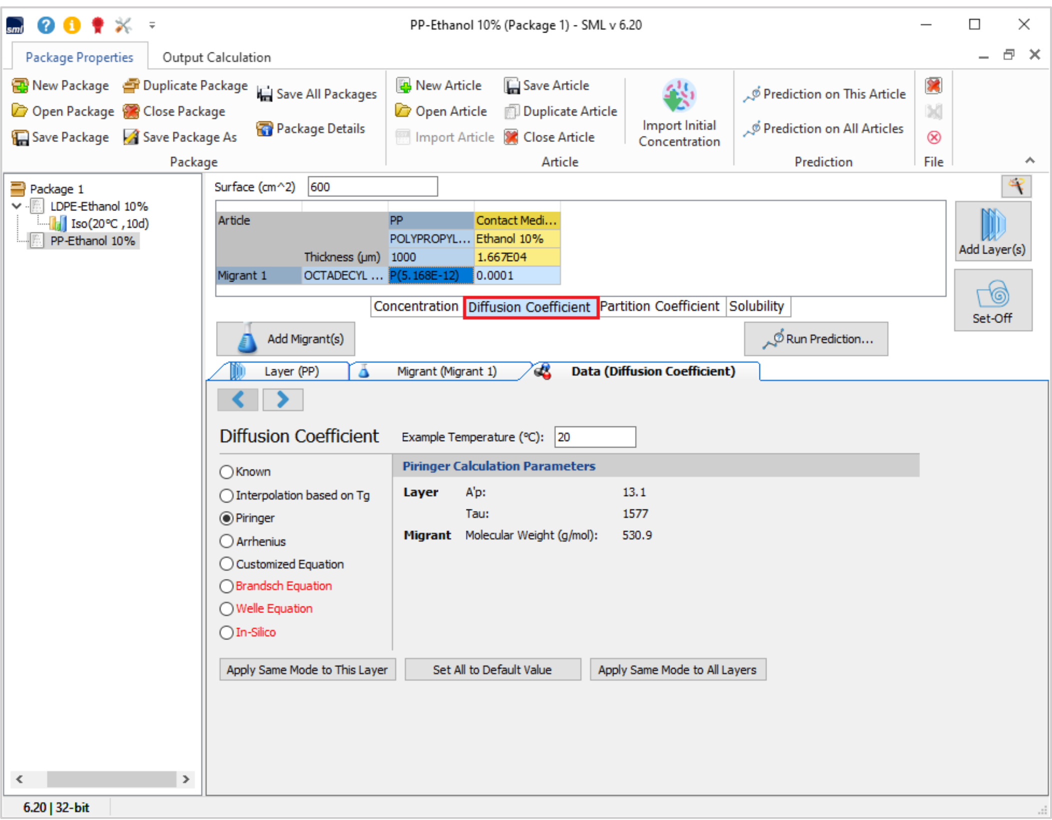


FIG. 13 - Diffusion coefficient will be automatically updated if estimation procedure is available (Methods highlighted in red cannot be chosen because of missing required parameters).

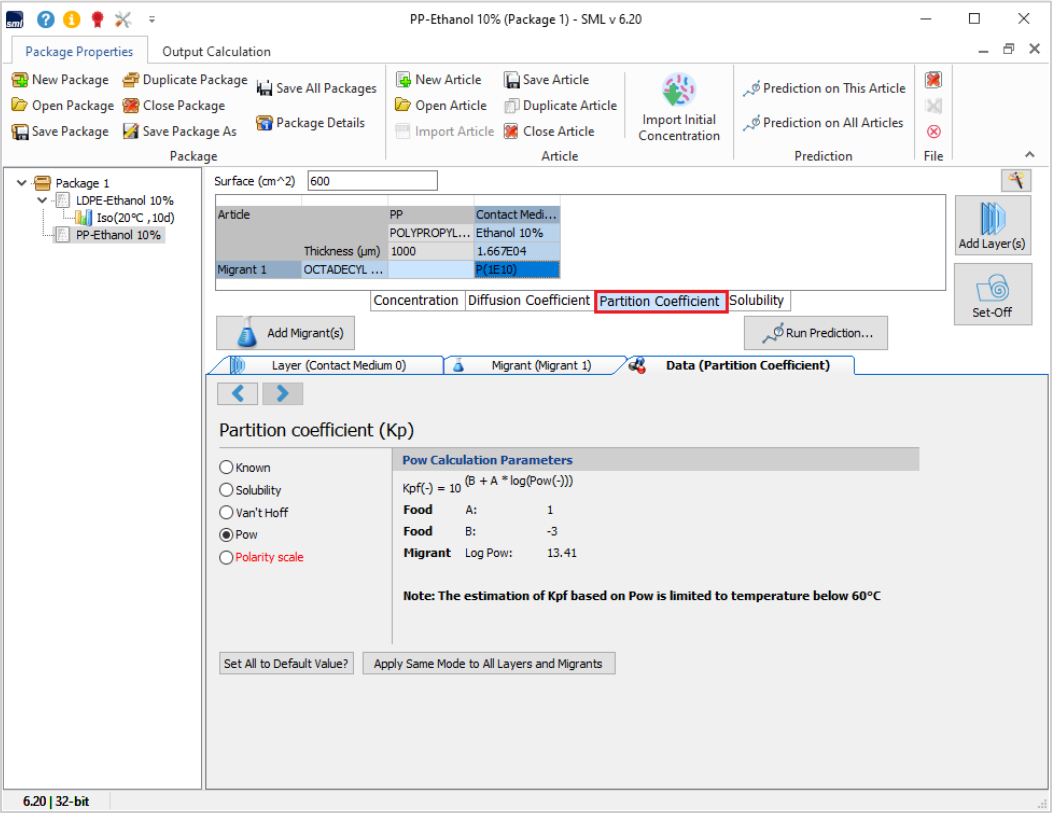


FIG. 14 - Partition coefficient will also be automatically updated if estimation procedure is available.

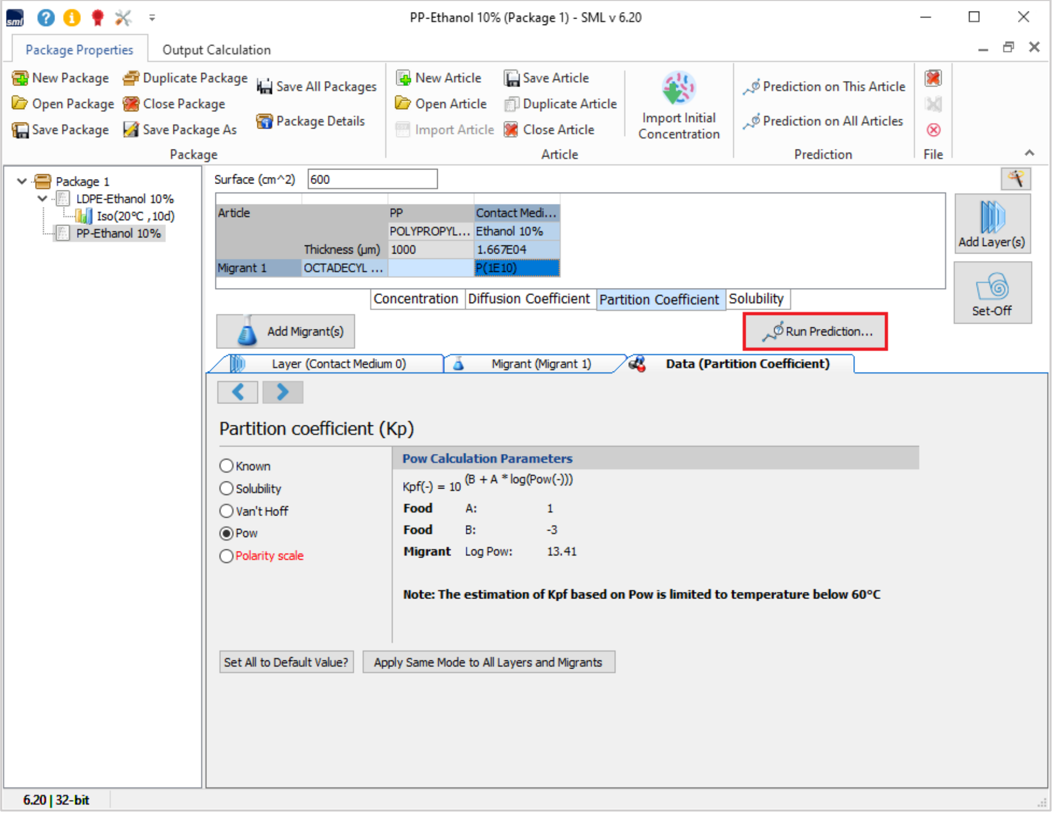


FIG. 15 - Migration calculation (click Run Prediction).

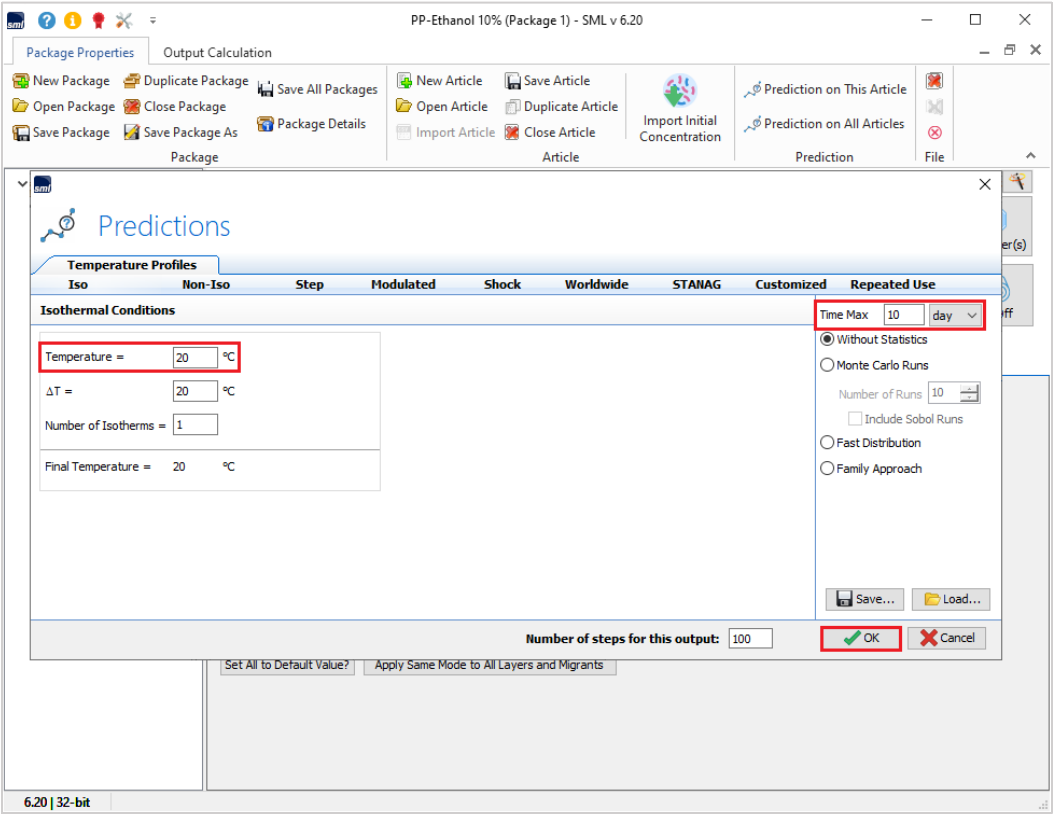


FIG. 16 - Prediction of migration of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) into the contact medium under isothermal conditions (here during 10 days at 20°C).

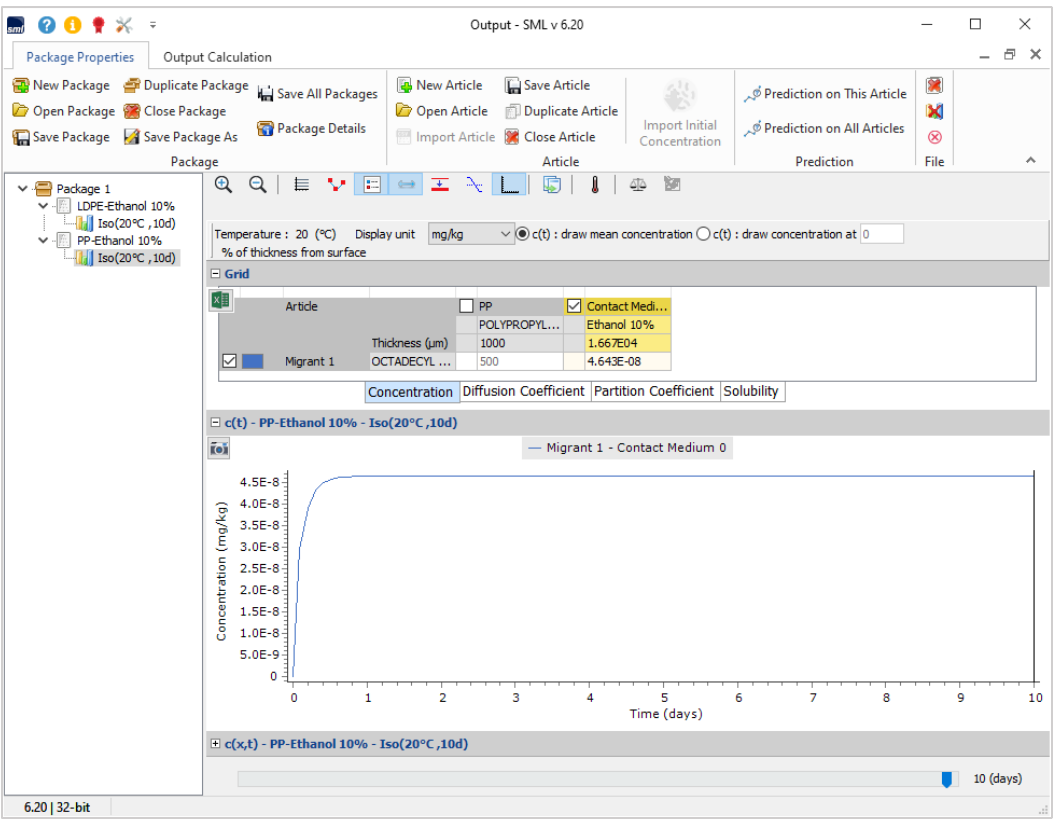


FIG. 17 - Concentration profile of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) over time to food simulant 'Ethanol 10%'. Note negligible concentration of migrant in food simulant being lower than 5E-8 mg/kg what indicates that the migration does not occur.

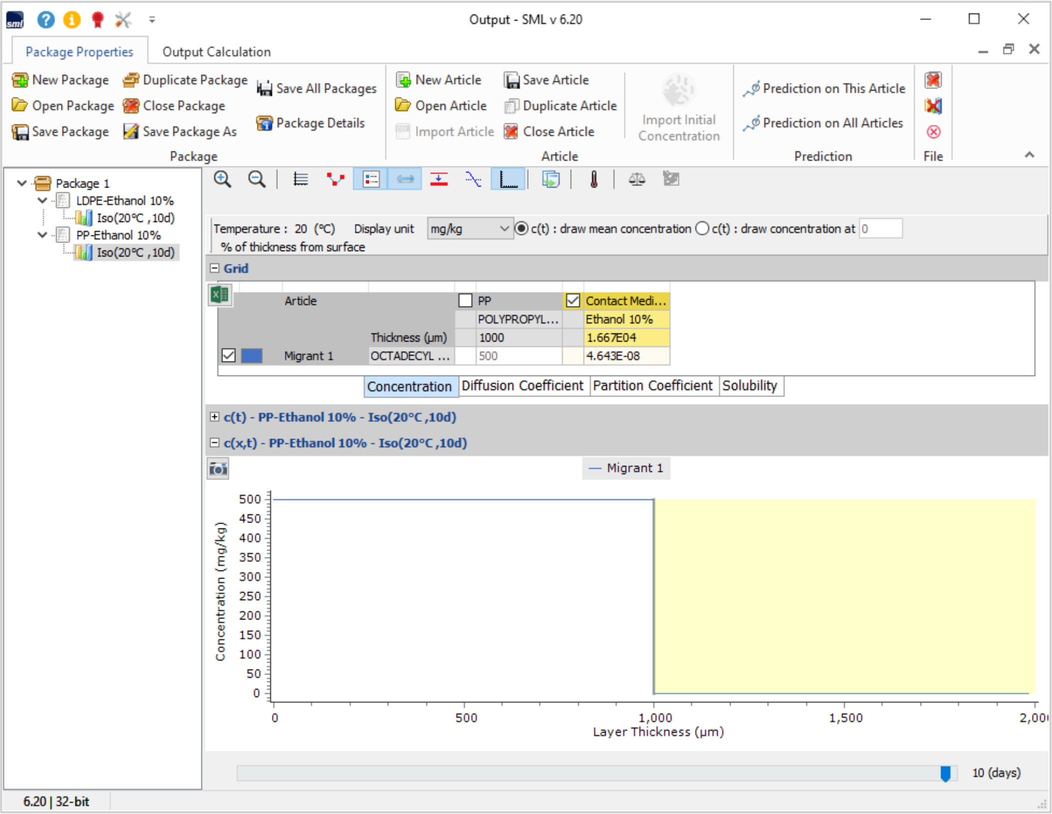


FIG. 18 - Concentration profile of migrant (Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate) over layer thickness and time, no migration to food simulant is observed.

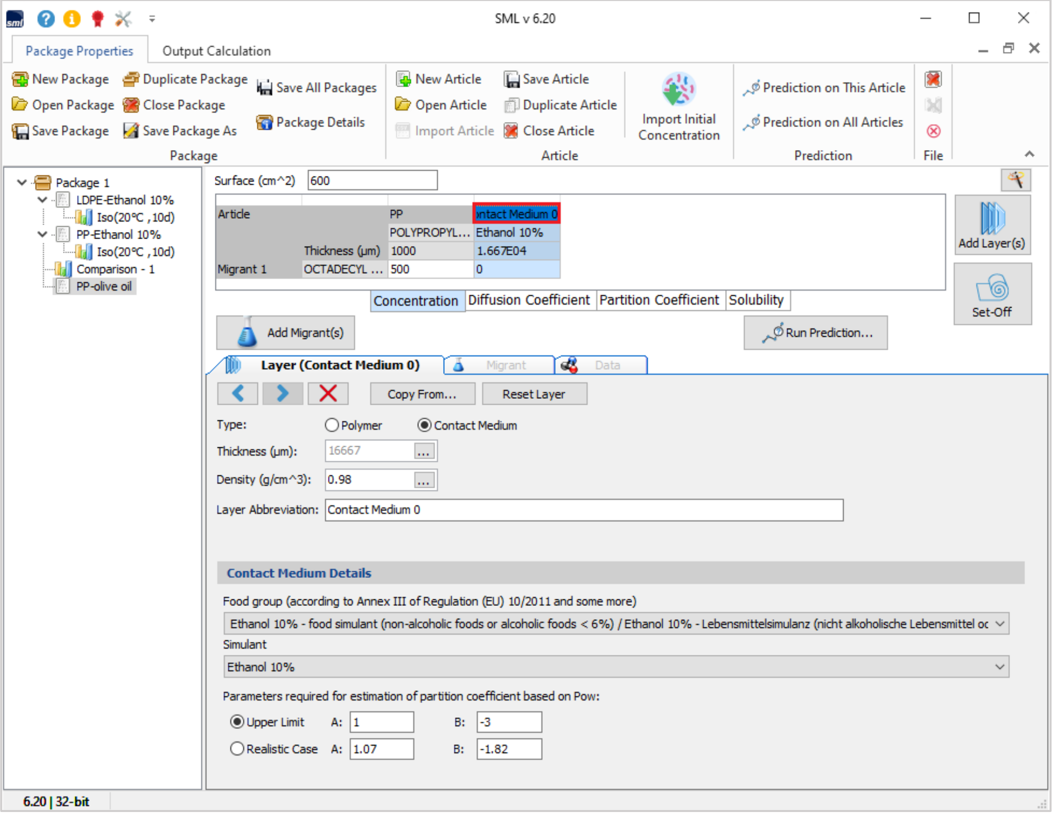


FIG. 19 - Changing the contact medium.

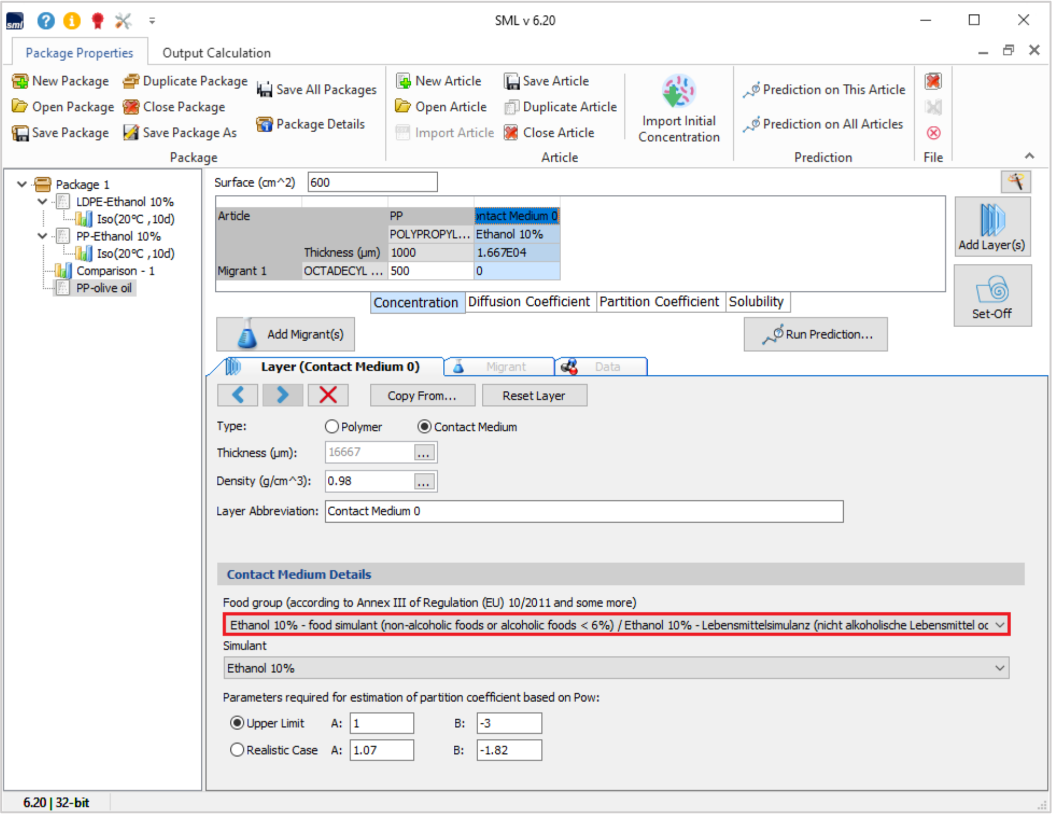


FIG. 20 - Selection of the food group (click on current food group).

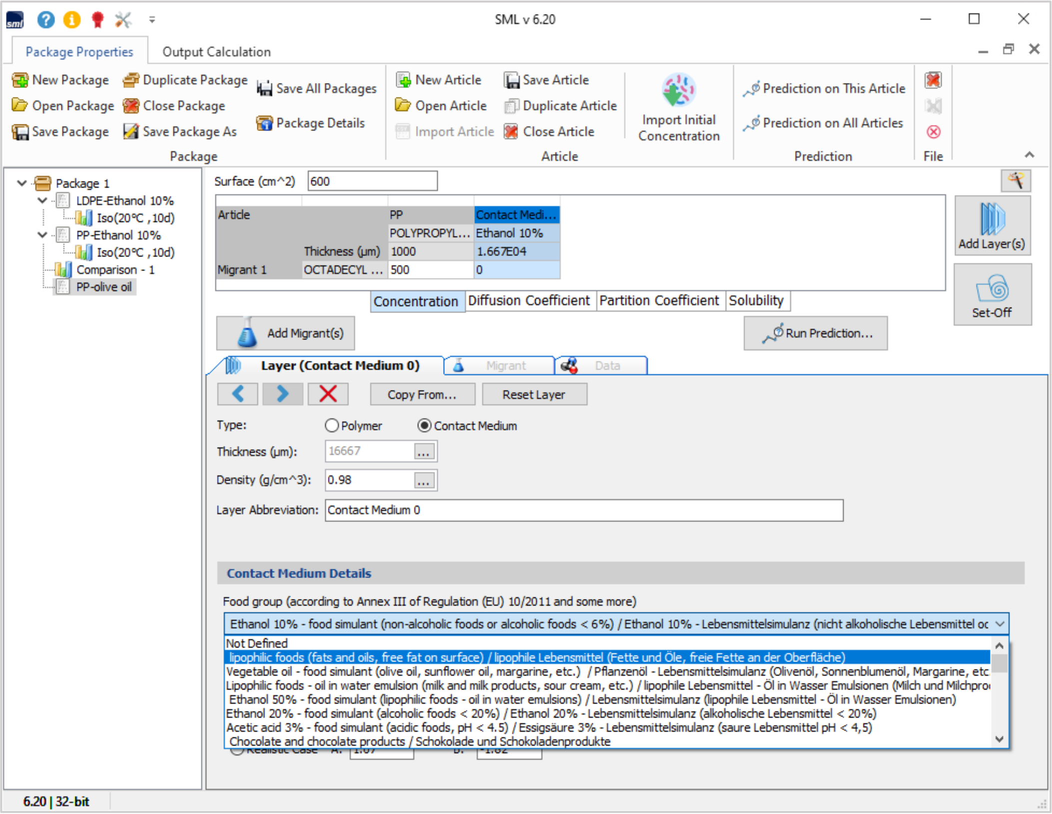


FIG. 21 - Changing the food group from 'Ethanol 10%' to 'lipophilic foods'.

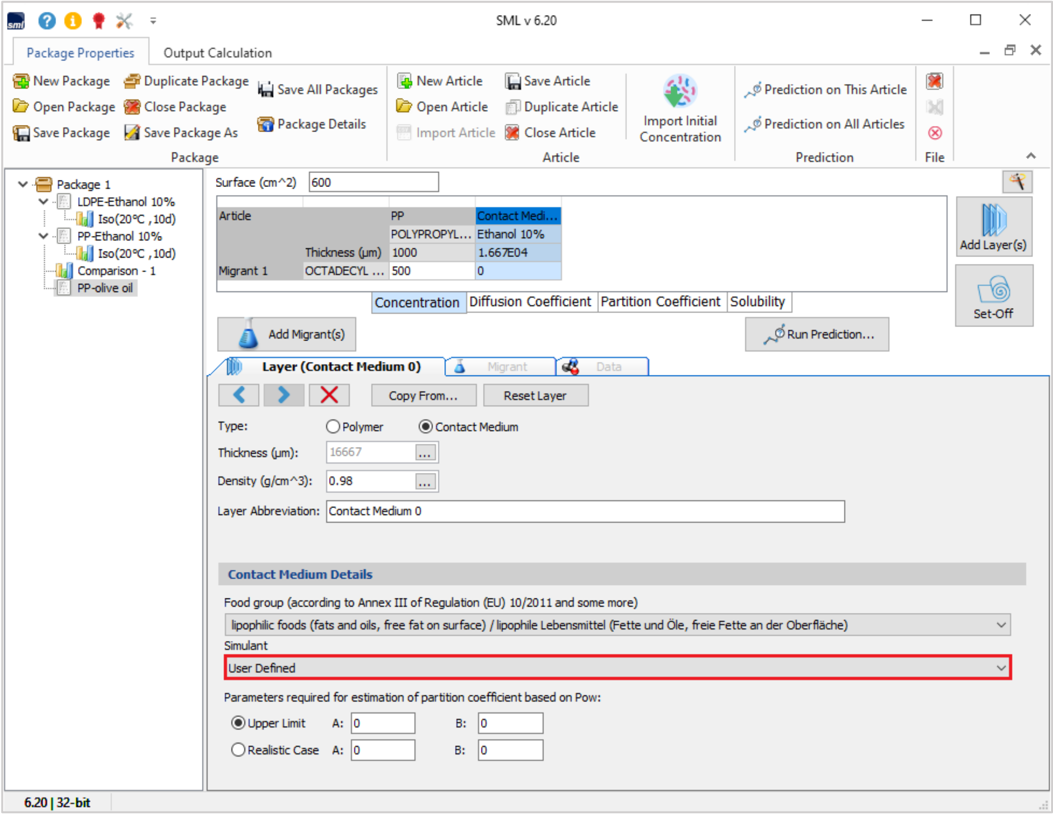


FIG. 22 - Selection of a food simulant.

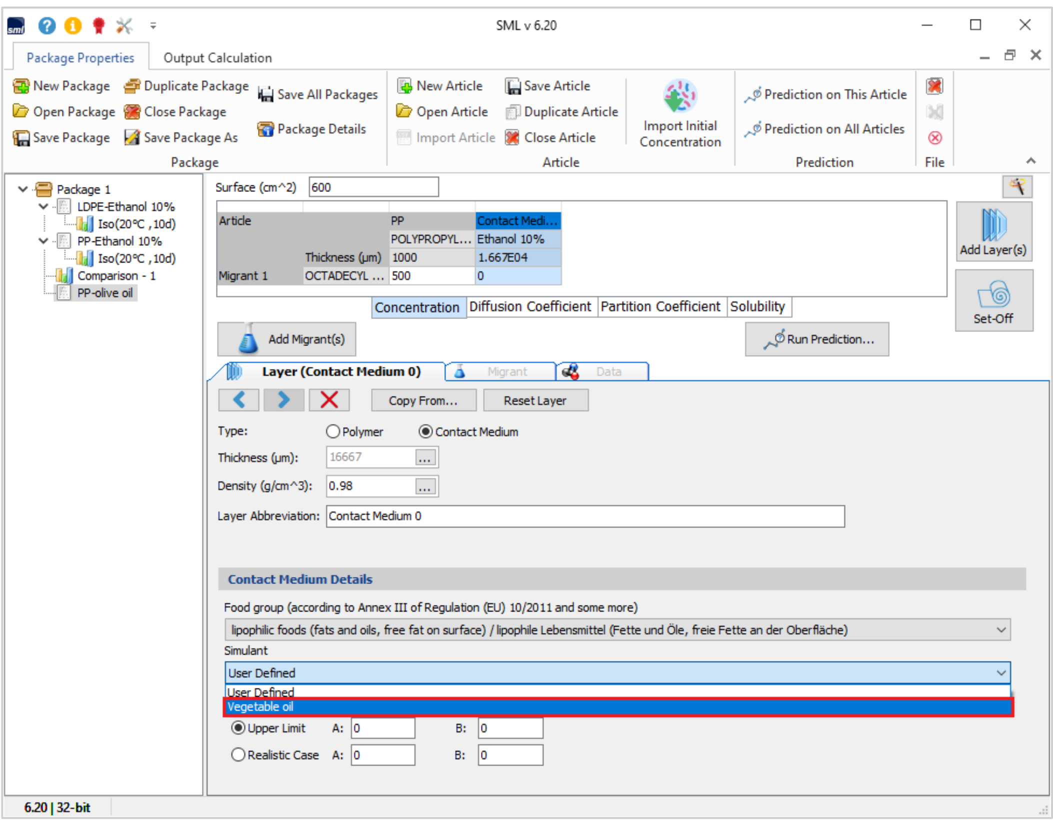


FIG. 23 - Selection of 'vegetable oil' as a food simulant.

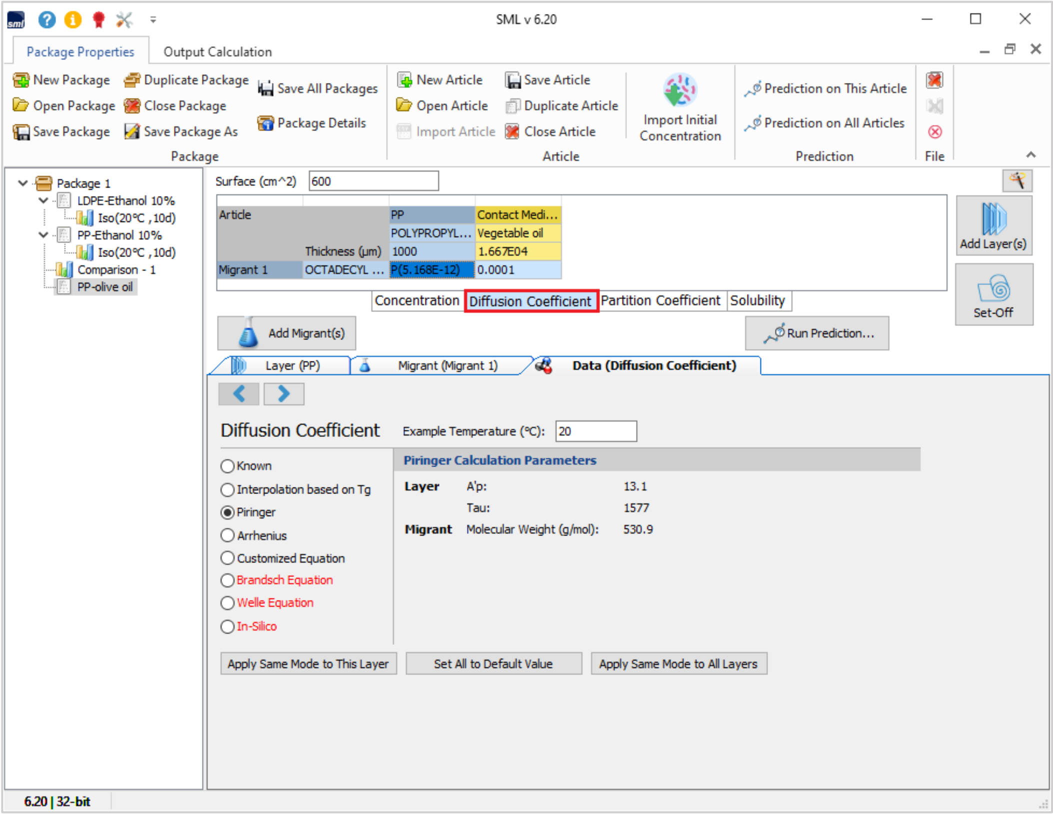


FIG. 24 – Evaluation of diffusion coefficient by Piringer method.

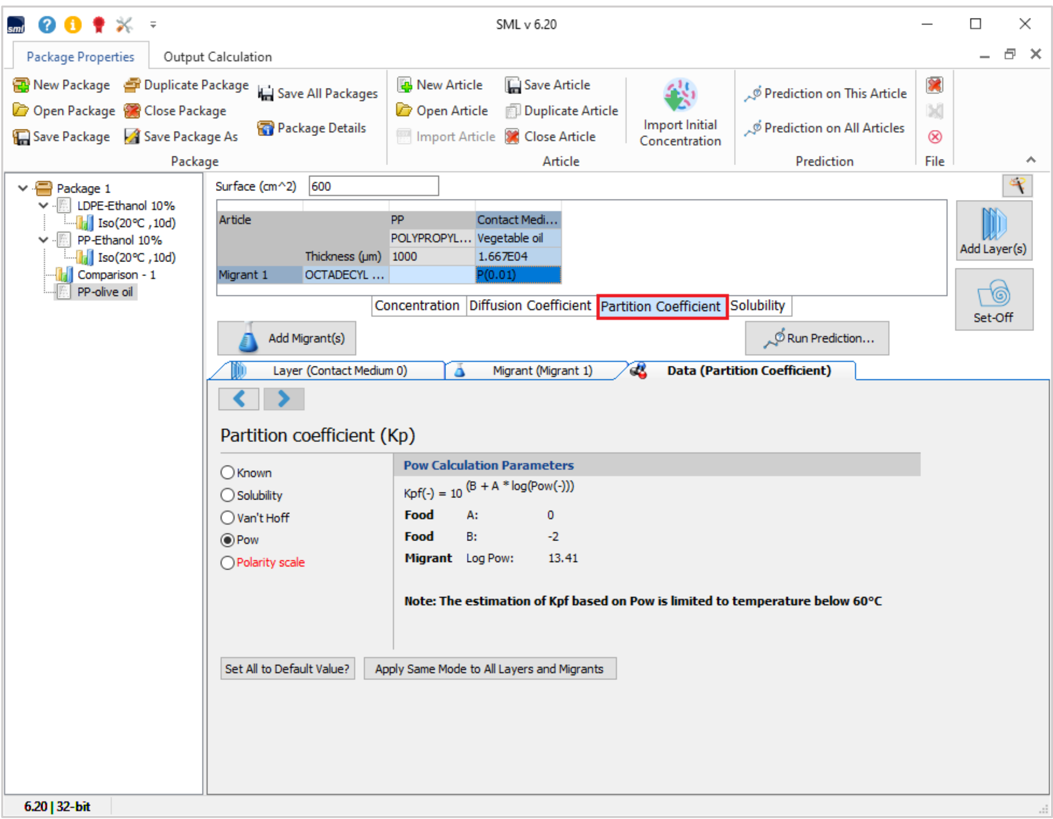


FIG. 25 – Evaluation of partition coefficient by Octanol/ Water method.

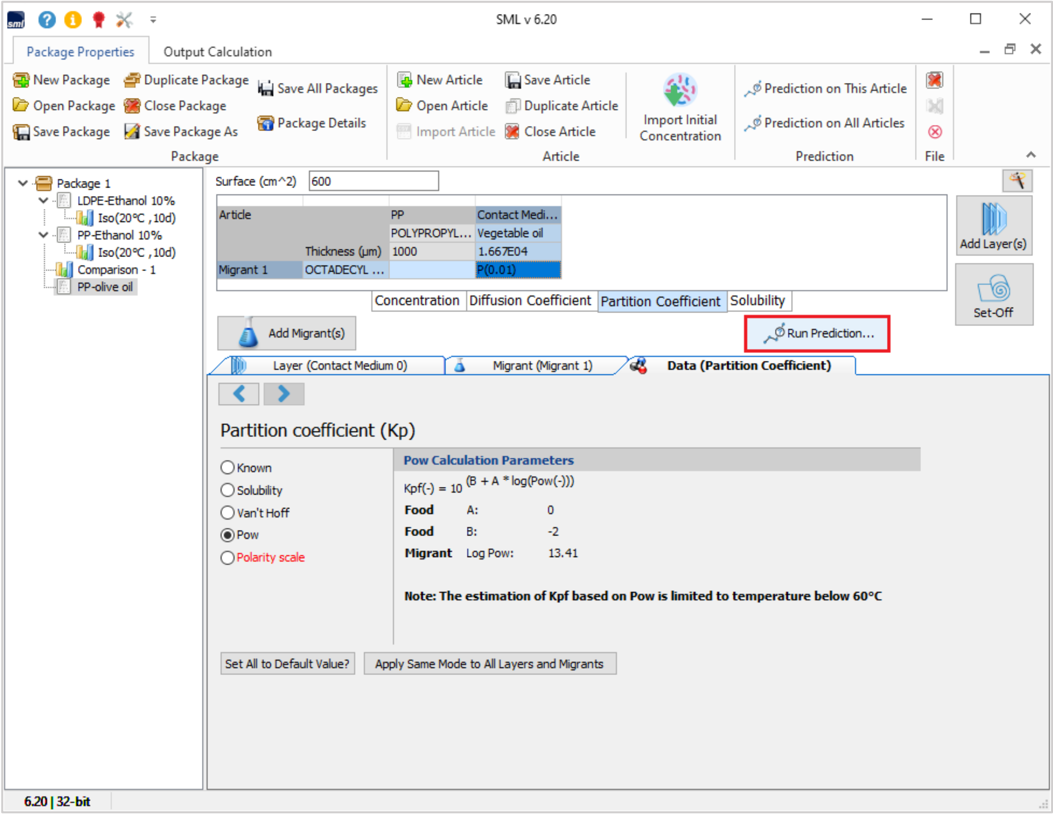


FIG. 26 - Migration calculation (click Run Prediction).

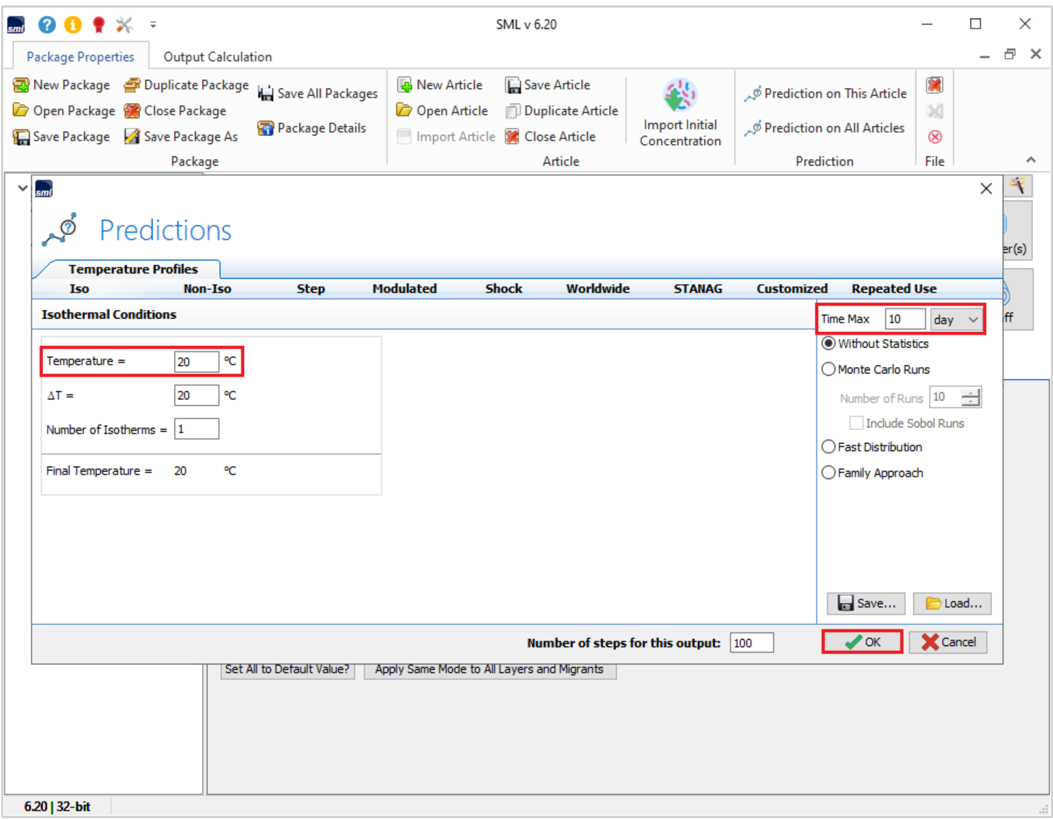


FIG. 27 - Prediction of migration under isothermal conditions (here during 10 days at 20°C).

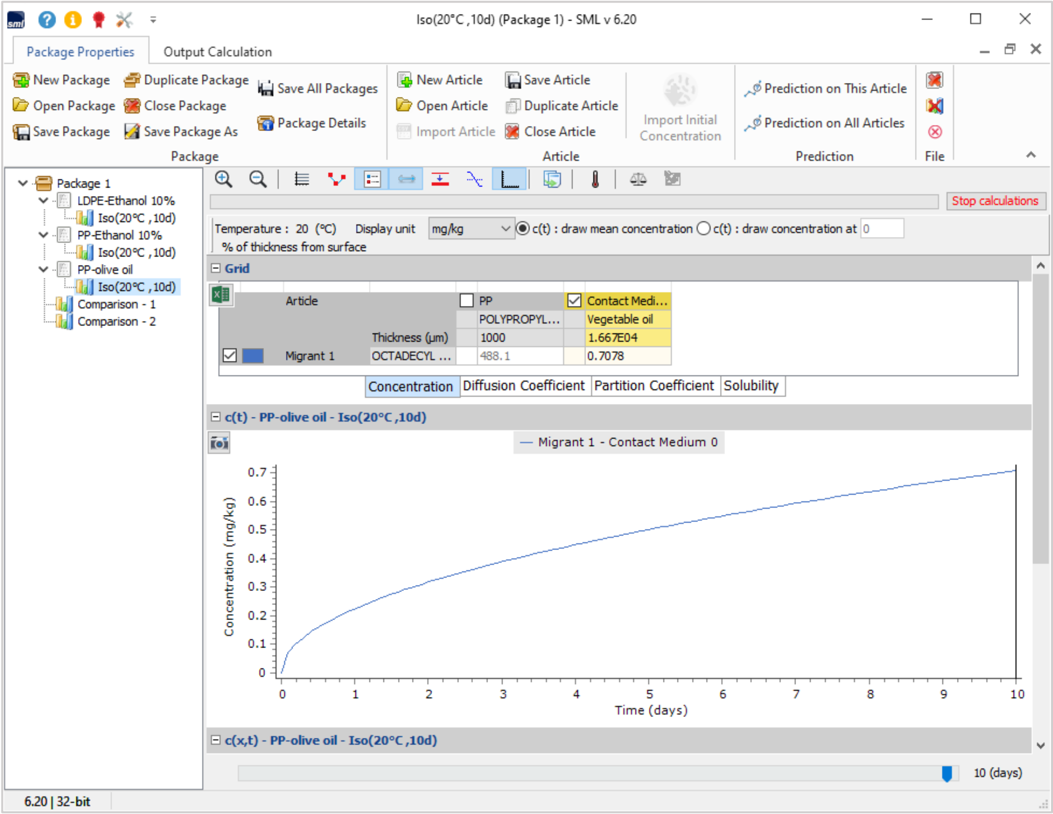


FIG. 28 - Migration profile of Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate over time in 'vegetable oil'. The significant migration takes place, note continuous increasing of concentration of migrant in olive oil.

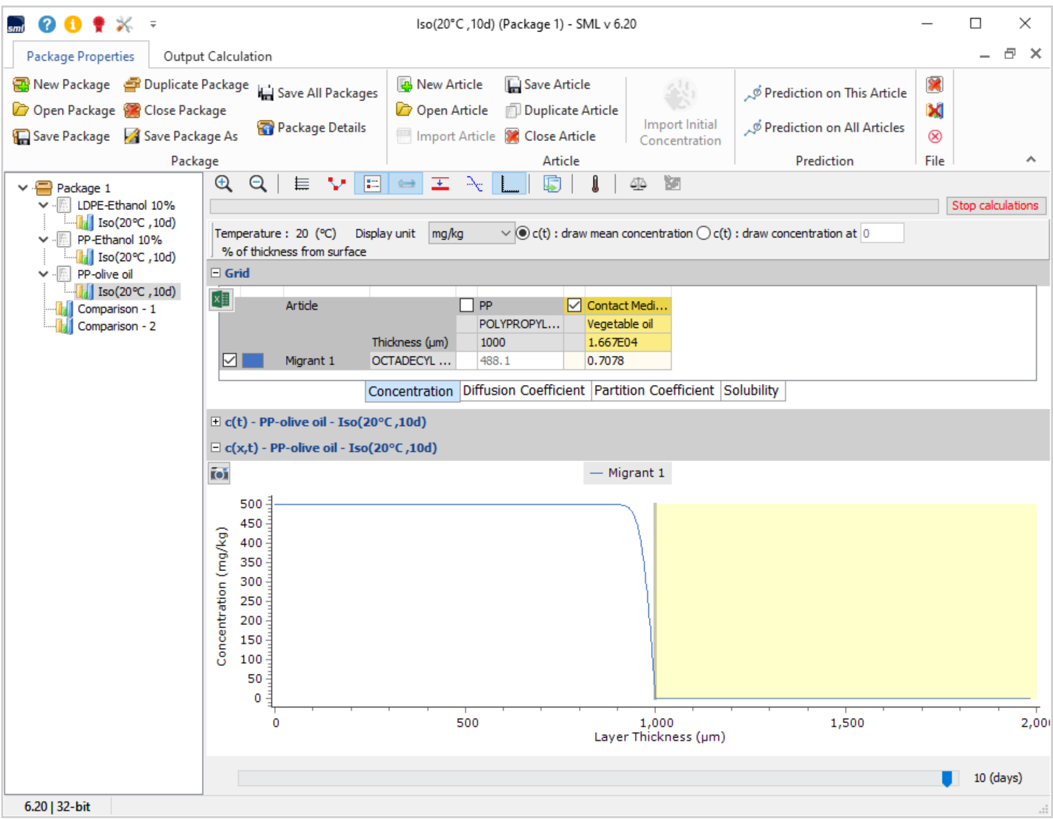


FIG. 29 - Migration profile of Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate over layer thickness and time in 'vegetable oil'. Displayed prediction indicates that migration takes place in 'lipophilic foods'.

RESULTS / COMPLIANCE CERTIFICATE

The output window shows the results of the simulated predictions. Following results may be displayed:

- The results grid
- The c(t) chart
- The c(x, t) chart
- Comparison Output
- Sum Output
- Compliance Certificate

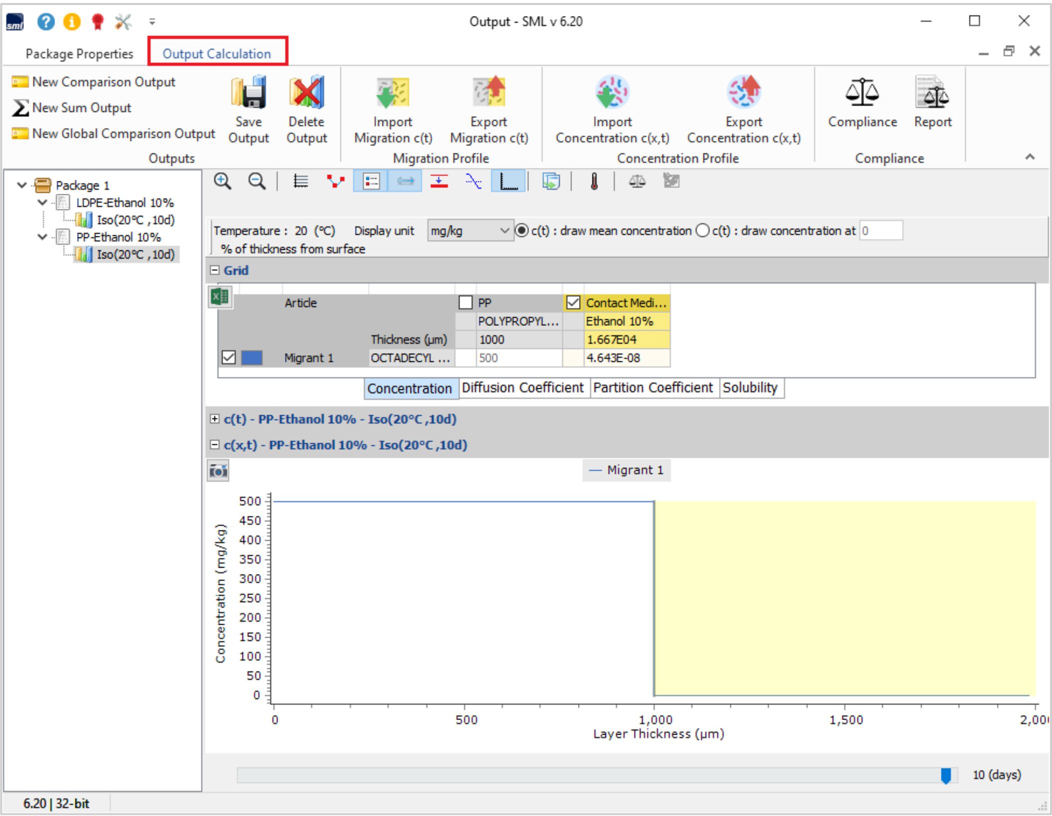


FIG. 1 - Selection 'Output calculation'.

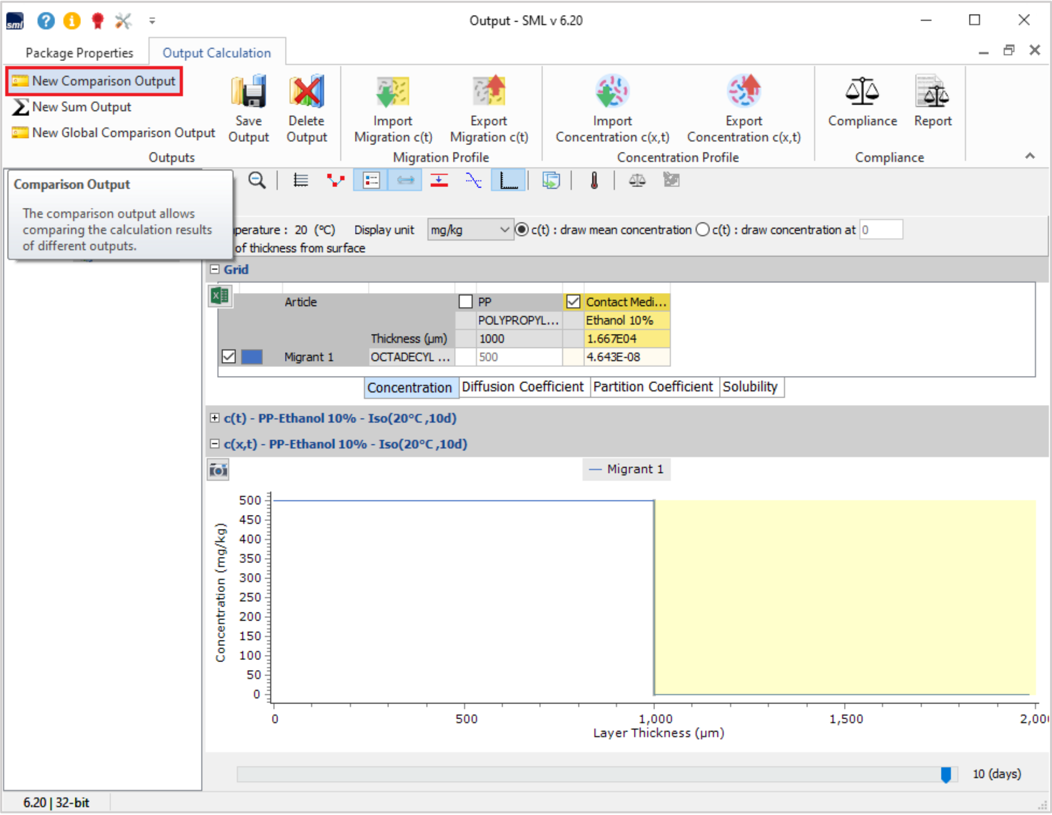


FIG. 2 - The 'comparison output' allows the comparison between migration profiles of Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate in layers of 'LDPE' and 'PP'.

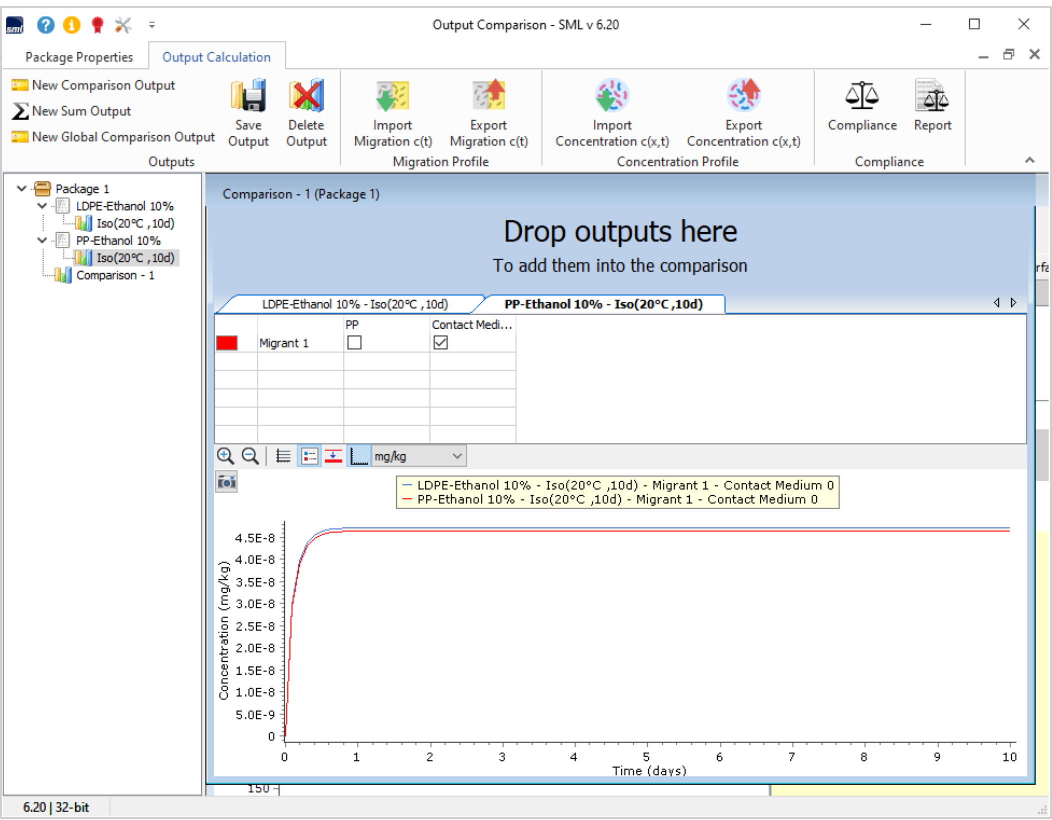


FIG. 3 - Migration results show no migration of migrant from both polymers ('LDPE' and 'PP') to food simulant 'Ethanol 10%'.

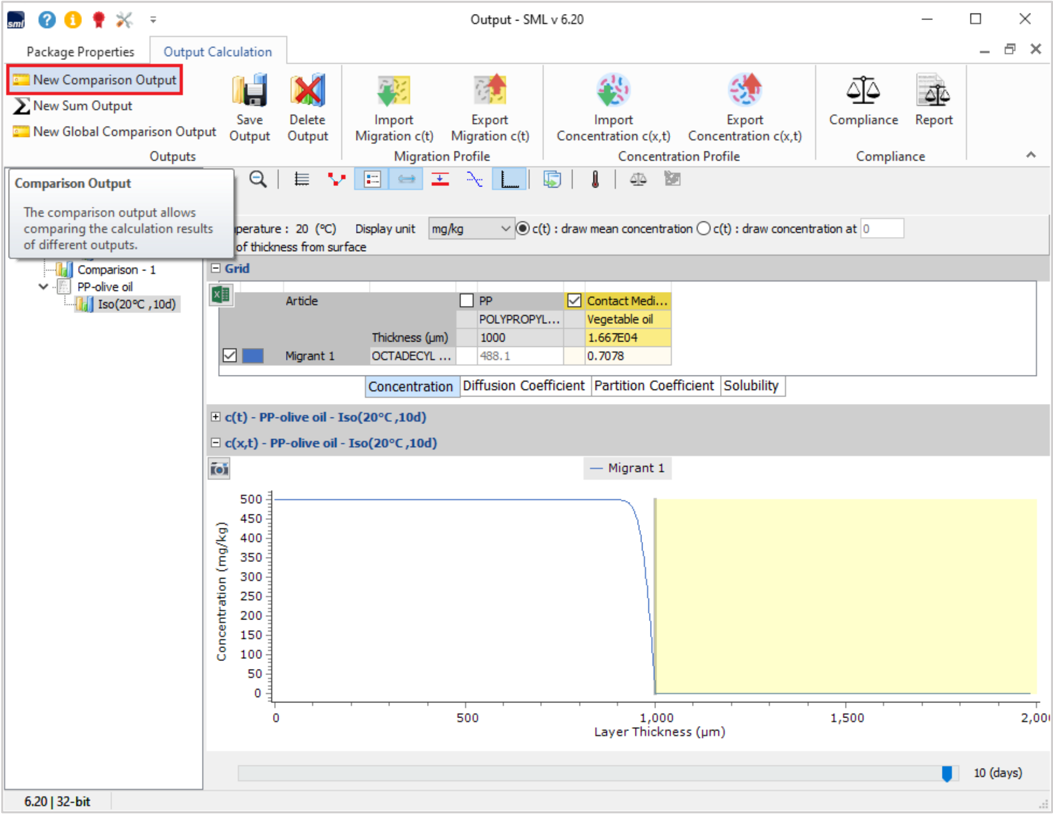


FIG. 4 - Selection of comparison output.

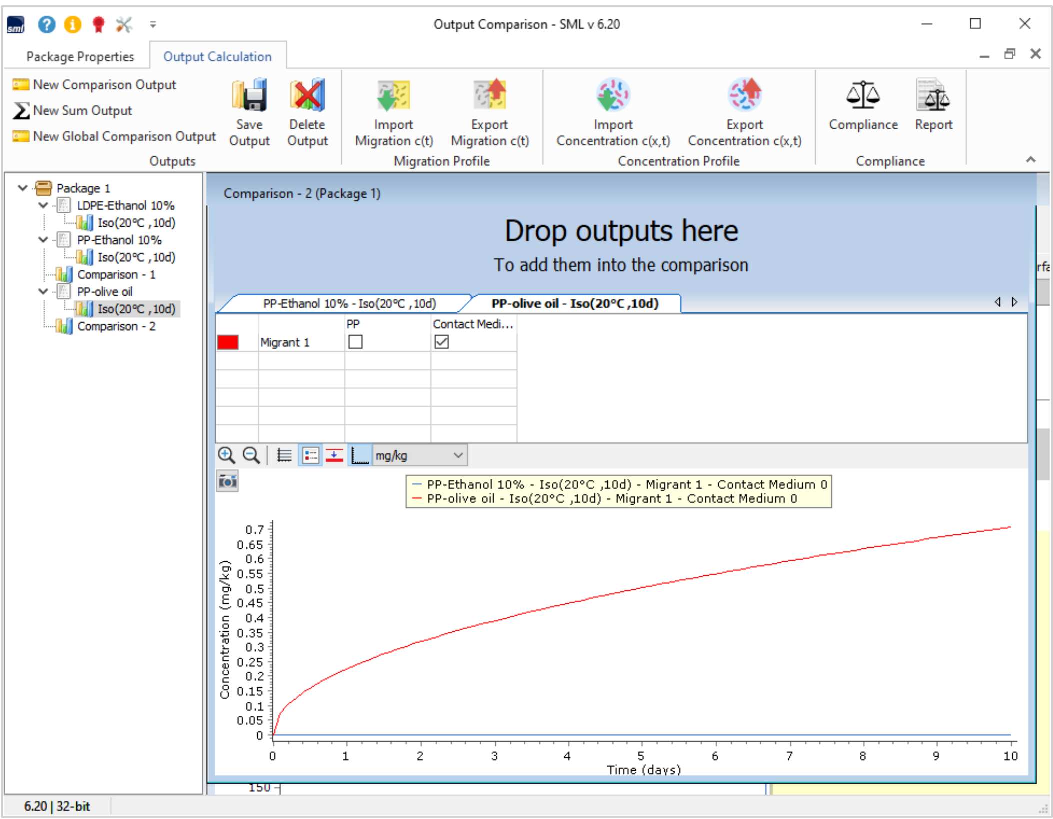


FIG. 5 - Migration profile over time for 'vegetable oil' (in red) and 'Ethanol 10%' (in blue). No migration is observed for ethanol solution.

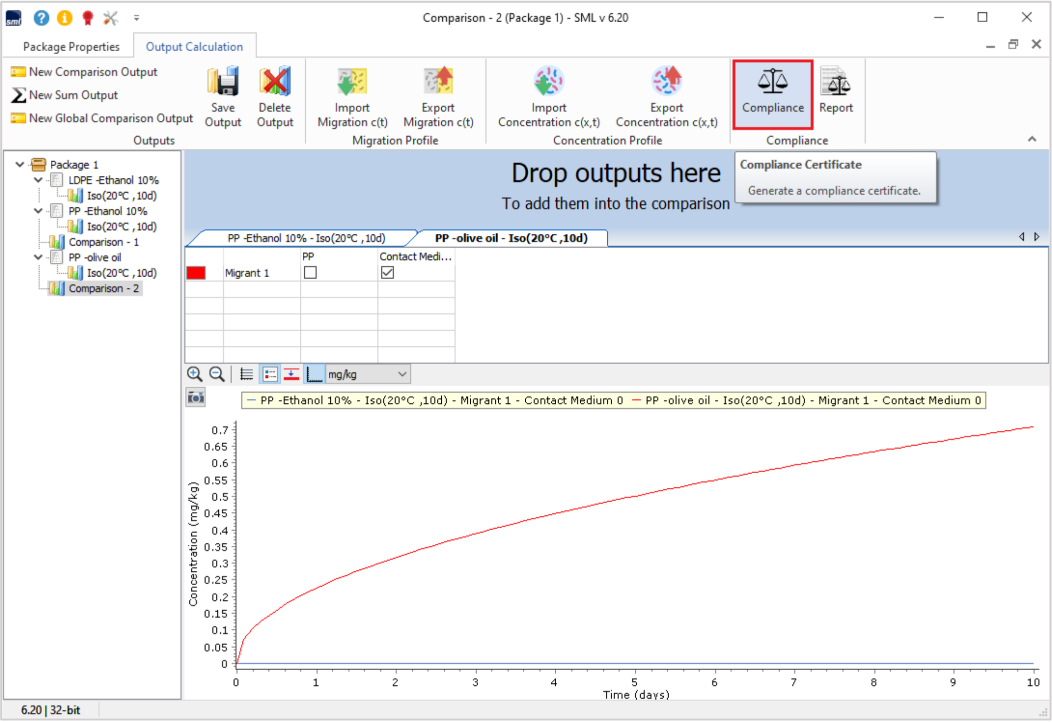


FIG. 6 - Click on 'Compliance' to generate the compliance certificate according to legislation conformity.

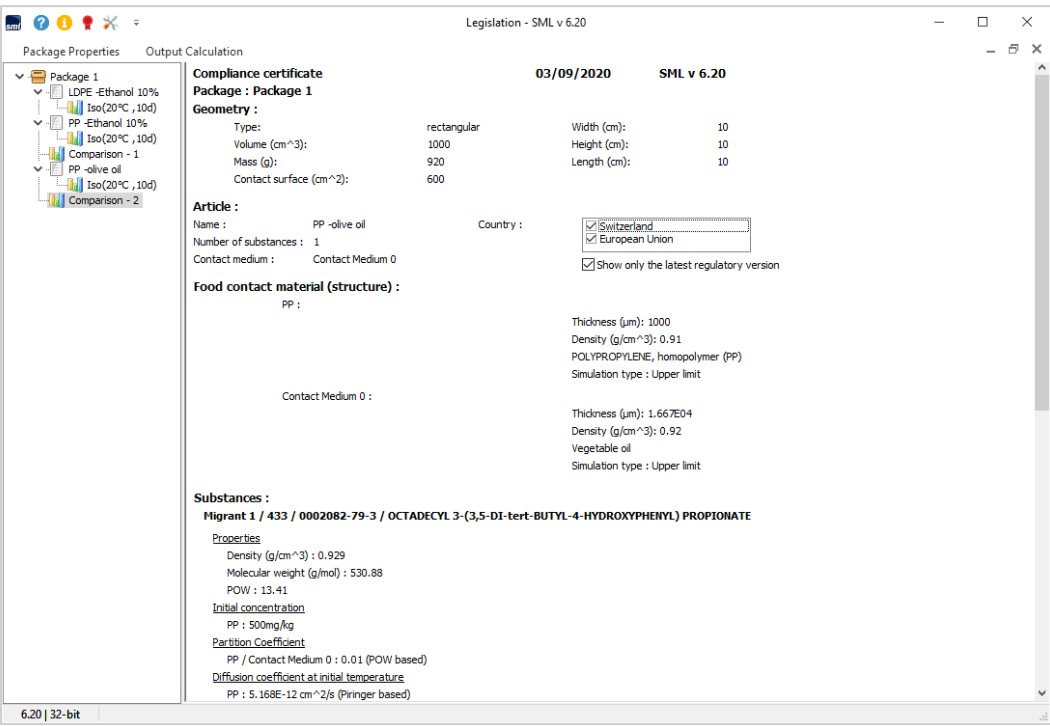


FIG. 7 - Compliance certificate for the system: polypropylene-olive oil- Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl) propionate.

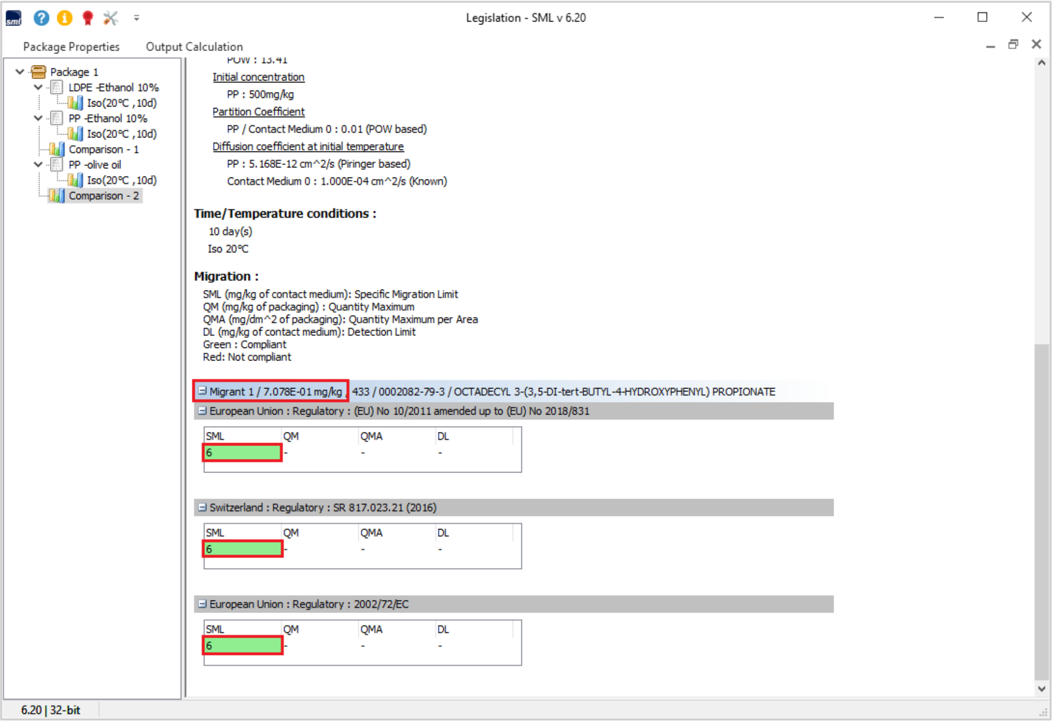
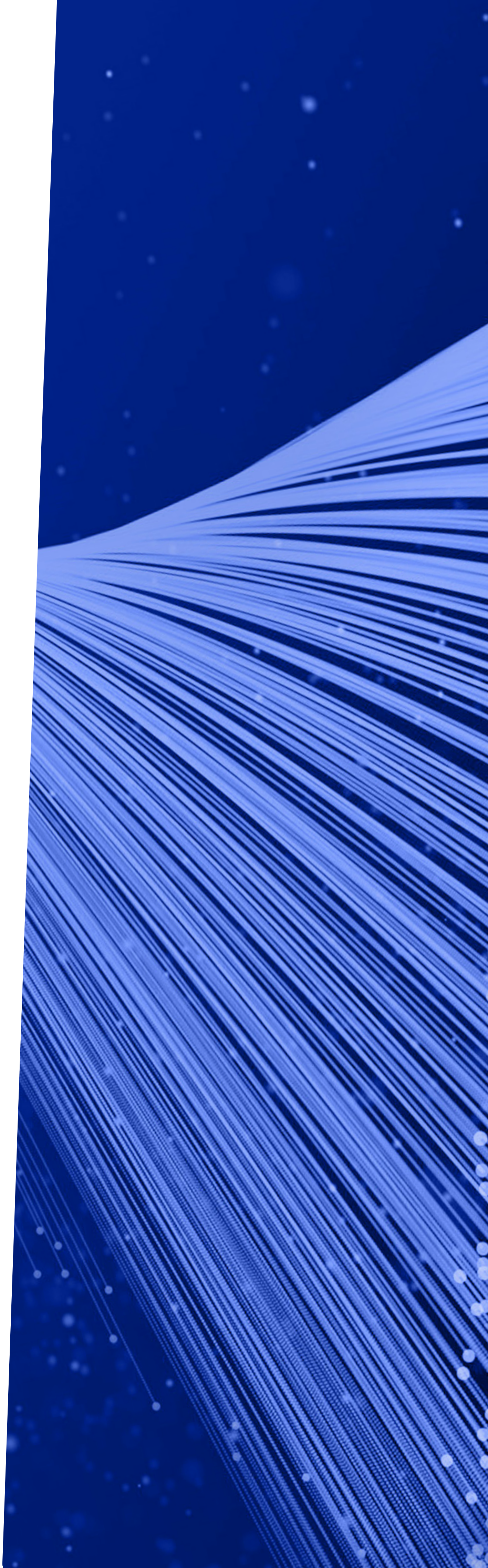


FIG. 8 - Compliance certificate: Comparison of migration calculation (7.078e-01 mg/kg) and food regulations (SML: 6 mg/kg) is marked in red. Green colour indicates that specific migration limit is not exceeded.

FOR FURTHER INFORMATION VISIT:
www.akts.com/sml



Phone +41 848 800 221
Email info@akts.com

AKTS SA
Technopôle 1
3960 Sierre
Switzerland