

Correlation of the solubility behavior for migrants of foods with ethanol-water mixtures and via $\log K_{PF}$ versus $\log P_{OW}$ relationships

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Introduction

Within the FACET project a convenient method for the determination of partition coefficients K_{PF} for migrants between polymer and food was developed. For this purpose 17 model migrants were selected to cover a wide range of physical-chemical properties (Table 2). With this method approx. 600 K_{PF} values between LDPE and FACET model foods (Table 1) were determined. Using the same method further migration tests were carried out using different ethanol concentrations (10, 20, 30, 40, 50, 60, 70, 80, 95%) and olive oil instead of foods to determine partition coefficients between the polymer and the food simulants (FS), $K_{PF/FS}$. $K_{PF/FS}$ data obtained from the Foodmigrasure project^[1] were also included to extend the data pool.

Method

First of all, the log-log-plot of partition coefficients between plastic and ethanolic solution ($K_{PF/FS}$) against octanol/water partition coefficients (P_{OW}) of the migrants was made and linear regression lines ("mean lines") were established. In this way a coordination system was established into which the results obtained from the food experiments, i.e. the $\log P_{OW}$ - $\log K_{PF}$ relationships were overlaid (Figure 1). Then to each FACET model food an ethanol-in-water equivalent was established (Figure 2). The physico-chemical meaning of this correlation is that when the log - log relationship (in form of a regression line) for a given food coincides with a given ethanol-in-water line then this food would have the same or similar solubility for migrants.

Table 1: FACET model foods and its water-ethanol equivalencies

FACET Model Foods	Ethanol-Equiv. [%]	FACET Model Foods	Ethanol-Equiv. [%]	FACET Model Foods	Ethanol-Equiv. [%]	FACET Model Foods	Ethanol-Equiv. [%]
Wine	20	Condensed milk	60	Noodles	35	Sausage: Polony	50
Apple sauce	25	Cottage cheese	40	Ground nuts	60	Pate	60
Orange juice	40	Soft cheese	50	Dough	95	Sausage: Salami	95
Ketchup	25	Whipping cream	95	Cake	70	Bacon	50
Tomato sauce	25	Cheese sauce	40	Buttertoast	50	Cooked ham	50
Milk powder	50	Gouda	60	Dark chocolate	95	Sausage: Landjäger	95
Instant soup	55	Yoghurt	50	Chocolate spread	75	Ham	50
Wheat flour	35	UHT milk	60	Honey	0	Pork raw	< 5 % fat: 30 5-20% fat: 40 > 20% fat: 50
Rice	45	Turkey	50	Margarine	95	Tuna	40
Mayonnaise	55	Salmon	40	Olive oil	95	Fish sticks	40

Table 2: FACET model migrants

FACET Model Migrants	
Diphenyl phthalate (DPP)	Benzophenone (BP)
Octadecyl-3-(3,5)-di-tert-butyl-4-hydroxyphenyl) propionate (Irganox 1076)	2,5-Bis(5-tert-butyl-2-benzoxazolyl) thiophene (Uvitex® OB)
2-Hydroxy-4-n-octyloxy-benzophenone (Chimasorb® 81)	1,4-Diphenylbutadiene (DPBD)
1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	Styrene
2,2-bis(4-hydroxyphenyl) propane (Bisphenol A)	1-Octene
Isopropyl thioxanthone (ITX)	Adipic acid, bis(2-ethylhexyl) ester (DEHA)
Triclosan	Tri-n-butyl acetyl citrate (ATBC)
	Diisopropyl naphthalene (DIPN)
	2,6-Di-tert-butyl-p-cresol (BHT)
	Diisononylphthalate (DINP)

Results

Using this approach allows in a new and pragmatic way to estimate K_{PF} values for any organic substance through its otherwise easily accessible P_{OW} value. Furthermore, based on this correlation the complete FACET food list with approx. 180 entries at the first tier (representing several thousands of individual foods at tier 3) can be assigned to ethanol-in-water equivalents and thus expressed as ethanol/water mixtures (Table 1).

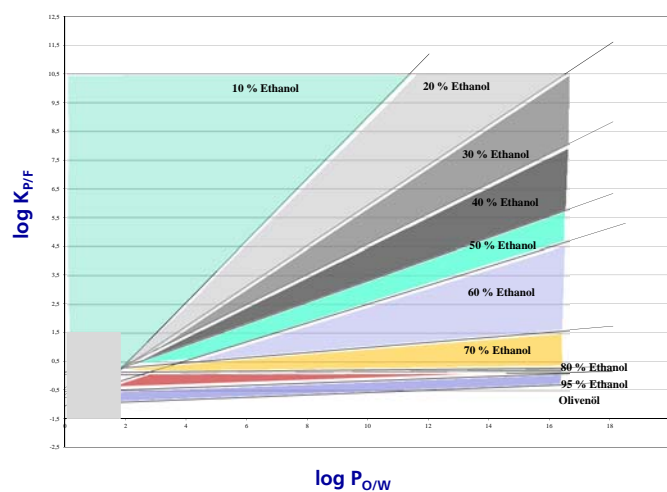


Figure 1: Coordination system ($\log P_{OW}$ - $\log K_{PF}$ relationship)

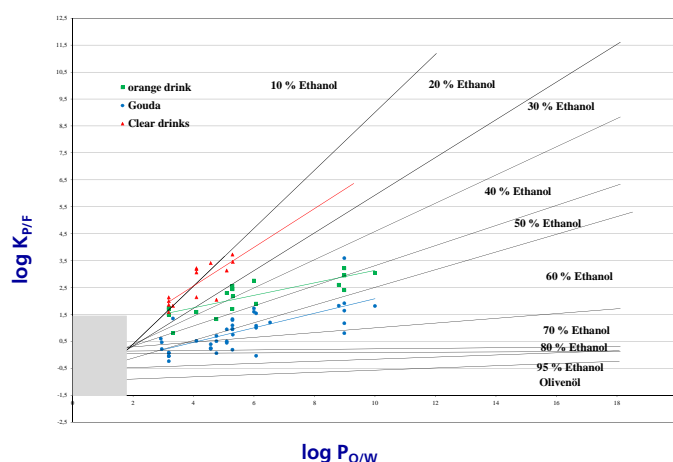


Figure 2: Correlation of water-ethanol equivalents to selected foods

Reference

^[1] FOODMIGROSURE project, contract number QLK-CT2002-2390