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Plastic Packaging Materials for Food

Barrier Function, Mass Transport, Quality Assurance, and Legislation

edited by O.-G. Piringer
and A. L. Baner

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Preface

One could say that this work was created in the laboratory but was born out of necessity. There has been a huge need for experimental data to support the harmonization of food packaging law in the European Union and to support the effort at streamlining approval of packaging materials coming into food contact in the United States.

Vast amounts of literature and data have been published containing the results of thousands of experiments measuring different interactions between polymers and contacting foods. This experimental data gathering has been accelerated in the past twenty years by continuous improvements in analytical equipment and the personal computer's ever increasing data handling abilities. The mathematical modeling of diffusion in polymers has been largely understood and was described over forty years ago in Crank's book "The Mathematics of Diffusion". Nevertheless, the frustration remained in many cases that one was still not able to model interactions in many cases using even the simplest diffusion equation because the necessary material constants were usually lacking.

The motivation for this book thus comes mainly from a desire to collect together in one place the current state of knowledge on interactions between polymeric materials and foods in package systems and then assemble this knowledge into a systematic approach that will allow estimation of the extent of these interactions. The end result it is hoped will be a practical guide to approximating and measuring the extent of interactions between polymers and foods.

In 1993 one of us (O. P.) wrote a book based largely on work carried out at the Fraunhofer-Institut für Lebensmitteltechnologie und Verpackung (Fraunhofer Institute for food technology and packaging) outlining a multi-disciplinary approach for estimating and measuring interactions between polymers and foods. However, in the intervening years it has been apparent that the book needed to be enlarged and updated to include numerous new developments. This new book not only starts where the previous edition left off but has been completely rewritten. Several authors specializing in the various fields covered in this book have agreed to contribute their expertise as it is no longer possible for one person alone to effectively cover the necessary material in the required depth.

The chapters in the first half of the book describe the basic fundamental knowledge about plastics, processing aids and additives as well as the physical-chemical and mathematical background of the mass transport in these systems. The second half of the book applies the information contained in the first half to the estimation, measurement and evaluation of polymer/food interactions. Foods are considered to be the "model substances" here but these findings can be applied to many other products and systems as well.

With a developing field such as this one, this book can only be a work in progress. The book does not try to be the last word on the subject and largely reflects the point of view and experience of its authors. It is hoped that the reader will find the information contained here practical and useful for understanding and estimating the phenomenon of polymer and food interactions and that researchers will be able to use this material as a starting point for future investigations.

The scientific literature which covers such a large interdisciplinary field uses a variety of symbols. In many cases different symbols are used to designate the same thing but the same symbol can be used also for completely different designations. This situation is also reflected in this book due to authors coming from many different countries and professional fields. To avoid confusion as much as possible a comprehensive list of all the symbols and many of the abbreviations used here has been prepared.

Reference lists are added at the end of each chapter reflecting the nature of the chapter being mainly a review or of a descriptive character. A comprehensive list of citations follows the large collection of diffusion coefficient values in Appendix I. In the first introductory chapter a list of useful secondary literature is given which contains many additional papers. Nevertheless, the authors are aware that many valuable references were not cited in this work.

Finally, we wish to thank the members of the staff at Wiley-VCH for all of their help and guidance.

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List of Abbreviations

Abbreviation	Description	Section
ADI	accetable daily intake (toxicological magnitude)	10.1.2
AFID	alkaliflame ionization detector	10.2.6
APCI	atmospheric pressure chemical ionization	10.2.6
API-MS	atmospheric pressure ionization – mass spectrometry	15.4
ASTM	American Society for Testing and Measurements	10.2.3
BCR	European Community Bureau of Reference	10.2.5
BGA	Bundesgesundheitsamt	3.1.6
BgVV	Bundesinstitut für gesundheitlichen Verbraucherschutz und Veterinärmedizin	10.1.2
CAS	Chemical Abstracts Service	10.2.6
CEN	European Committee for Standardization	10.1.2
DIN	Deutsche Industrie Normen	10.2.3
DST	dual sorption theory	5.1
EC	European Community	10.1.2
EC	electro conducting	3.1.4
EDI	estimate of daily intake	11.2
EEC	European Economic Community	10.1.2
EN	European Standard	10.1.2
ENV	European Prestandard	10.1.2
EPA	Environmental Protection Agency	10.2.3
ESI-MS	electron spray ionization – mass spectrometry	15.4
ESIPT	exited state intramolecular proton transfer	3.2.2
EU	European Union	10.1.2
FAO	UN Food and Agriculture Organization	10.2.3
FB	functional barrier	10.3.2
FDA	Food and Drug Administration (USA)	10.2.3
FID	flame ionization detection	10.2.6
FP	food packaging	10.2.6
fs	femtosecond = 10^{-15}s	5.2.1
FVP	functional validation and precision	10.2.6
GC	gaschromatography	10.2.2
GC/FID	gaschromatography/flame ionization detector	10.1.2

Abbreviation	Description	Section
GC/MS	gaschromatography/mass spectrometry	10.2.2
HPLC	high performance liquid chromatography	15.3
HSGC/FID	headspace gaschromatography/flame ionization detector	10.2.6
ILSI	International Life Sciences Institute	10.3.3
ISO	International Organization for Standardization	10.2.3
LC	liquid chromatography	10.2.6
LMBG	Lebensmittel- und Bedarfsgegenständegesetz	10.2.6
LOD	limit of detection	10.2.2
MAFF	Ministry of Agriculture Foods and Fisheries	10.2.6
MC	Monte Carlo method	5.2
MD	molecular dynamics	5.2
MS	mass spectrometry	10.2.4
MSD	mean-square displacement	5.2.1
ns	nanosecond = 10^{-9}s	5.2.2
OM	overall migration	10.2.6
PM/Ref	European packaging material reference number	10.2.6
ps	picosecond = 10^{-12}s	5.2.1
QM	maximum quantity (toxicological magnitude)	10.1.2
QM(T)	maximum permitted quantity of the residual substance in the material or article expressed as total of moiety or substances indicated	10.2.6
R	recycling-related	10.3.2
R&D	research and development	10.3.2
RIM	reaction injection moulding	2.3.1
SATP	standard ambient temperature and pressure	9.1.1
SCF	Scientific Committee of Food	10.2.5
SFC	supercritical fluid chromatography	10.2.6
SIM	selective ion monitoring	10.2.6
SM	specific migration	10.1.2
SML	specific migration limits (toxicological magnitude)	10.1.2
SRM	single reaction monitoring	10.2.6
STP	standard temperature and pressure	9.1.1
TDI	tolerable daily intake (toxicological magnitude)	10.1.2
TRC	threshold-of-regulation-concentration	10.3.2
TSA	transition-state approach	5.2
TST	transition-state theory	5.2.2
UNIFAC	UNIfied quasi chemical theory of liquid mixtures Functional-group Activity Coefficients	4.3.2
UNIFAC-FV	Unifac free volume	4.3.2

List of Chemical and Polymer Abbreviations

Abbreviation	Description	Section
ABS	acrylonitrile-butadiene-styrene	2.3.1
aPP	atactic polypropylene	5.2
BADGE	bisphenol-A-diglycidyl ether	2.1.1
BHT	butylated hydroxytoluene	11.4
BOPP	biaxially orientated polypropylene	2.3.1
Box	2-benzoxazolinone	10.2.6
BR	butadiene rubber	2.3.1
BS	butadiene-styrene	10.2.6
CR	chloroprene rubber	2.3.1
DAA	diacetone alcohol	13.3.5
DAS	9,10-dimethoxyanthracene-2-sulphonic acid	10.2.6
DEG	diethyleneglycol	10.2.6
ECH	epichlorohydrine	10.2.6
EDA	ethylenediamine	10.2.6
EP	epoxide resins	2.3.1
EPDM	ethylene-propylene-diene rubber	2.3.1
EVA	ethylvinylacetate	2.3.1
EVOH	ethylvinylalcohol	2.3.1
GPPS	general purpose polystyrene	14.1
HAS	hindered amine stabilizers	3.1.7
HB 307	mixture of synthetic triglycerides	11.4
HD	hydroperoxide-decomposing antioxidant	3.2.3
HDPE	high density polyethylene	2.3.1
HIPS	high impact polystyrene	2.3.1
HMDA	hexamethylenediamine	10.2.6
IPS	impact polystyrene	2.3.1
IR	isoprene rubber	2.3.1
LDPE	low density polyethylene	2.3.1
LLDPE	linear low density polyethylene	2.3.1
MEG	monoethyleneglycol	10.2.6
MEK	methylethylketone	13.3.2
MeOH	methanol	10.2.6
MF	melamine-formaldehyde resins	2.3.1
MPPO	modified polyphenylene oxide	Tab.(12–10)
NBR	acrylonitrile-butadiene rubber	2.3.1
OPA	biaxial streched polyamide	2.3.1
OPP	oriented polypropylene	2.3.1
P4MP1	poly(4-methylpentene-1)	2.3.1

Abbreviation	Description	Section
PA	polyamide	2.3.1
PAI	polyamideimide	5.2.1
PBT	polybutylene terephthalate	2.3.1
PC	polycarbonate	2.3.1
PCL	polycaprolactone	2.3.1
PDA	propylenediamine	10.2.6
PDMS	polydimethylsiloxane	5.2
PE	polyethylene	2.3.1
PEG	polyethyleneglycol	10.3.4
PES	polyethersulfone	2.3.1
PET	polyethyleneterephthalate	2.3.1
PF	phenolic resins	2.3.1
PHB	poly-D(–)-3-hydroxybutyric acid	2.3.1
PHV	polyhydroxyvalerate	2.3.1
PI	polyimide	5.2.1
PIB	polyisobutylene	2.3.1
PMMA	polymethylmethacrylate	2.3.1
PO	polyolefins	2.3.1
POM	polyoxymethylene	2.3.1
PP	polypropylene	2.3.1
PPS	polyphenylsulfide	2.3.1
PS	polystyrene	2.3.1
PSU	polysulfone	2.3.1
PTFE	polytetrafluorethylene	2.3.1
PUR	polyurethane	2.3.1
PVC	polyvinylchloride	2.3.1
PVDC	polyvinylidenechloride	2.3.1
QM	quinone methide	3.2.2
SAN	styrene-acrylonitrile	2.3.1
SB	styrene-butadiene	2.3.1
SBR	styrene-butadiene rubber	2.3.1
TBA	tribromoanisole	13.3.4
TCA	trichloroanisole	13.3.4
THF	tetrahydrofurane	10.2.6
UF	urea-formaldehyde resins	2.3.1
UP	unsaturated polyester resins	2.3.1
VCM	vinylchloride monomer	Tab. (12–1)
VDC	vinylidenechloride	2.3.1
VLDPE	very low density polyethylene	2.3.1

List of Symbols

Latin symbols

Symbol	Description	Section
a	activity	4.1.2
a	solute radius	6.1
a	ratio of food volume to volume of polymer	11.4
a (x,y,z)	scalar field	7.1.1
a,b	correlation constants for molecular weight and temperature effects on diffusion	11.5
a,b,c	chemical components	4.1.1
a_c, a_r, a_{fv}	components of activity represent combinatorial, residual and free-volume contributions	4.3.2
a_l	Langmuir capacity constant, in Eq. (5–8), [cm^3(STP)/cm^3 polymer atm]	5.1.2
A	free energy	4.1
A	surface of revolution area of particles	6.2.1
A	surface area	7.1.1
A	integration constant	7.2.3
A	matrix with tridiagonal structure	8.2.2
A	constant, determined from experimental data	11.5
A_d	diffusion model parameter, in Eq. (5–6), [$cm^2 \cdot$ mole/J $\cdot$ s]	5.1.1
A_m	molar cross-sectional area of the diffusing particle	6.4.1
A_p	effect of the polymer on diffusivity	11.5
A'_P	athermal term of the polymer on diffusivity	15.1.1
A(r)	Helmholtz energy, [J]	5.2.2
A_r	relative atomic mass (weight)	4.2
A_u	unit area	6.4.1
b	hole affinity constant, in Eq. (5–8), $[atm]^{-1}$	5.1.2
b	parameter account for the specific contributions of the migrant	15.1.1
B	propagation matrix	8.2
B	scattering between the laboratories	10.2.3
B_d	diffusion model parameter, in Eq. (5–6)	5.1.1
c	concentration	7.1.3
c	parameter account for the specific contributions of the diffusion activation energy	15.1.1

Symbol	Description	Section
c_a	concentration of permeant at time t in external phase	9.3.2
c_e	total concentration of permeant in polymer at echilibrium	9.3.1
c_i	concentration of component i in food	1.1
c_s	concentration of penetrant in polymer, in Eq. (5–5), [g/g polymer]	5.1.1
c_t	concentration of permeant in plastic at time t	9.3.2
$c_{F,e}$	concentration at equilibrium of a migrant in foodstuff or food simulant	10.1.1
$c_{F,t}$	average concentration of the odor compound in the outer layer of the food, having a thickness $d_{F,t}$	13.5
$c_{F,t}$	concentration of migrant in food at time t	14.3.3
$c^*_{F,t}$	estimated concentration of migrant in the food	14.3.3
$c_{F,0}$	initial concentration of migrating component in food simulant	10.1.1
$c_{F,\infty}$	concentration of migrant in the food at echilibrium	14.3.1
$c_{G,a}$	molar concentration of "a" in the gas phase	4.1.2
$c_{L,a}$	molar concentration of "a" in liquid	4.1.2
c_P, c_F, c_G	concentration of a substance in the packaging material, food and gas	13.4
$c_{P,a}$	molar concentration of "a" in a polymer	4.1.2
$c_{P,e}$	concentration ratio at equilibrium of a migrant in polymer	10.1.1
$c_{P,0}$	initial concentration of migrant in polymer	10.1.1
c'_H	hole sturation constant, in Eq. (5–8), [cm^3(STP)/cm^3polymer]	5.1.2
c'_P	mass of substance per unit surface area of packaging	13.5
$c'_{P,max}$	maximum allowable amount of an odor substance in a packaging material	13.5
$\bar{c}$	term defined in Eq. (6–2)	6.1
c_{11}	cohesive energy density in a pure liquid (1)	4.3.1
Δc	concentration gradient	7.2.9
Δc_i	concentration change	5.1
C	local concentration of penetrant in polymer, in Eq. (5–8), [cm^3/cm^3polymer]	5.1.2
CrD_{95}	critical difference of two group of measurements (y_1 and y_2)	10.2.3
CF	consumption factor	10.3.1
d	diameter of penetrant molecule (particle) [cm]	5.1.1
d	thickness of film	7.2.1
d_{eff}	effective "diameter" of nonspheric penetrant, [cm]	5.1.1
d_l	longest molecular dimension of penetrant, [cm]	5.1.1
$d_{F,t}$	average penetration distance of the solvent into the food up to time t	13.4
d_P	layer thickness of polymer	10.1.1
D	mutual or apparent diffusion coefficient, [cm^2 /s]	5.1.1
D_o	parameter in Eq. (15–2)	15.1.1
D_a	diffusion coefficient in amorphous polymer	9.1.3
$D_{c\to o}$	diffusion coefficient at "zero" penetrant concentration, [cm^2/s]	5.1.1
D_e	diffusion of the solute in the external phase (food)	11.4

Symbol	Description	Section
D_P	diffusion coefficient in the polymer	6.4.3
D_u	unit value of diffusion coefficient	6.1
D_F	diffusion coefficient of odor compound in food	13.4
D_G	gas self diffusion coefficient	6.1
D_L	diffusion coefficient in liquid	6.1
D_P^*	"upper bond" value of the diffusion coefficient which is larger than any possible real D_P for the migrant	15.1.1
$D_{P,i}, D_{P,j}$	diffusion coefficients of additive i respectively of simulant j in polymer	10.1.1
D_S	diffusion coefficient in solid	6.1
D_T	thermodynamic diffusion coefficient, [cm^2/s]	5.1.1
D_o	constant pre-exponential factor, in Eq. (5–7), [cm^2/s]	5.1.1
D_{1s}	solvent self-diffusion coefficient, in Eq. (5–7), [cm^2/s]	5.1.1
D^*	intradiffusion (tracer) coefficient	6.4.1
D^+	intrinsic diffusion coefficient, [cm^2/s]	5.1.1
e	random deviation in results occuring in every measurement	10.2.3
erf(z)	error function	7.2.3
E	environment	1.2
E	sum of all molecular increments	4.2
E_A	molar activation energy	6.4.1
E_b	intramolecular energy term, [kJ/mole]	5.1.1
E_d	activation energy of diffusion, [kJ/mole]	5.1.1
E_D	activation energy of diffusion	9.1.1
E_i	intermolecular energy term, [kJ/mole]	5.1.1
E_i	value of structural increment "i"	4.2
E_P	activation energy of permeation	9.1.1
E^*	critical energy, in Eq. (5–1), [kJ/mole]	5.1
E^+	energy per mole to overcome attractive forces from neighbors, in Eq. (5–7), [kJ/mole]	5.1.1
ΔE	theoretical activation energy of diffusion, in Eq. (5–4), [kJ/mole]	5.1.1
f	number of degrees of freedom involved in a diffusional jump, in Eq. (5–1)	5.1.1
f	flow rate	9.1.2
f_D	correction term	6.1
f_T	food type distribution factors	11.2
F	food (food simulating liquid)	1.2
F	force	6.4.1
g	system's mass	4.1.3
g_a	mass of component "a"	4.1.3
g_i	mass of component "i"	4.3.2
G	free enthalpy (Gibbs free energy)	4.1

Symbol	Description	Section
G	number of different groups present in mixture	4.3.2
G	gas	4.1.1
$\underline{G}$	molar free enthalpy	4.1
G_A	total free enthalpy of two separate liquids	4.1.1
G_E	total free enthalpy of the mixture (Gibbs free energy)	4.1.1
G^E	excess free energy	4.1.2
h	Planck constant = $6.626 \cdot 10^{-34}$ J · s	
h	spatial mesh constant	8.2
H	enthalpy	4.1
H	Henry's law constant	4.1.1
$\underline{H}^E$	excess enthalpy of mixing per mole	4.1.2
ΔH_S	molar heat of solution of gas in polymer	9.1.1
ΔH_v	molar enthalpy of evaporation	6.3.3
$\Delta \underline{H}_{v,1}$	molar enthalpy of vaporization (liquid 1)	4.3.1
i	migrating component	7.2.4
J	contribution of flux	7.1.1
J	flux vector	7.1.1
k	Boltzmann constant =$1.38. 10^{-23}$ J/K	
k	reaction rate constant	7.1.3
k	spatial wave number	8.2.1
k	proportionality factor	10.1.1
k*	transmission factor in Eq. (5–11)	5.2.2
K	partition coefficient	4.1.1
K	constant, determined from experimental data	11.5
K	parameter in Eq. (15–2)	15.1.1
k_D	solubility parameter in Henry's law, in Eq. (5–8), [cm^3(STP)/cm^3 polymer · atm]	5.1.2
$K_{G/F}$	partition coefficient of a migrating compound between gas and food	13.4
$K_{G/P}$	partition coefficient of a migrating compound between gas and packaging material	13.4
$K_{P,F}$, $K_{P/F}$	partition coefficient of a migrating compound between the plastic ,P, and the foodstuff or simulating liquid ,F	10.1.1 , 13.4
K_{12} and K_{22}	free volume parameters of the polymer, in Eq. (5–9), [cm^3/ g · K]	5.1.2
l	length	9.1.2
l	thickness of material	14.3.5
l_L	thickness of Nernst diffusion layer	7.2.5
l_P	thickness of packaging material	14.3.1
l_{12}	correction factor for cohesive energy density in a mixture of two substances (1+2)	4.3.1
L	liquid (liquid food)	4.1.1
L	thickness of sheet	8.2

Symbol	Description	Section
L	length	9.1.2
L_P	thickness of polymer	11.4
m	mass quantity	7.1.1.
m	mass of a particle	6.1
m	average of all values for the material studied (characteristic level)	10.2.3
m_e	amount of gas absorbed	9.1.2
m_E	mass transport from environment of package into food	1.2
m_F	mass transfer from food into package and environment	1.2
m_F	mass of food	13.5
$m_{F,e}$	amount of a substance migrating from polymer into food (simulant) at echilibrium	10.1.1
$m_{F,t}$	amount of a substance migrating from polymer into food (simulant) at time t	10.1.1
$m^*_{F,t}$	estimate migration amount	15.1.1
m_P	mass transport from package into food	1.2
m_P	mass of packaging	13.5
$m_{P,t}$	amount of a substance migrating into polymer from food or simulant during the contact time t	10.1.1
m^*	mass of backbone element, in Eq. (5–4), [g]	5.1.1
M	molar mass (mole)	4.1.3
M	number of spatial gridpoints	8.2
M_a	molar mass of component "a"	4.1.2
M_e	molecular retention index	4.3.3
M_i	concentration of migrant in the i-th food simulating solvent	11.2
M_r	relative molecular mass	2.2.1
$M_{t,\infty}$	mass that migrates at infinite time	11.4
M_w	relative molecular weigth, [dalton]	5
$M_{F,t}$	mass of solute that migrates at time t	11.4
$M_{F,\infty}$	mass of solute that migrates at infinite time	11.4
M_P	relative molar mass of monomeric structural unit	4.1.3
MW	relative molecular weight	11.5
M_1	molecular weight of solute	4.3.2
$M_2^{(m)}$	molecular weight of unit of polymer	4.3.2
n	number of different components	1.1
n	number density of molecules in mixture	6.1
n	order of reaction	7.1.3
n	time step index	8.2.1
n_i	number of a given type of increment	4.2
$n_a(L)$	quantity of material in liquid	4.1.2
n_1,n_2	number of measurements	10.2.3
N	Avogadro number= $6.022 \cdot 10^{23}$ [molecules/mole]	