

## Modeling Dynamic Flavor Release from Water

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A mathematical model derived from the convective mass transfer theory was developed to predict dynamic flavor release from water. A specific mass transfer correlation including a new term for volatile permeability was applied. The model was entirely based on physicochemical constants of flavor compounds and on some parameters of an apparatus used for validation. The model predicted a linear pattern of release kinetics during the first 30 s and large differences of absolute release for individual compounds. Both calculated and experimentally determined release profiles of a test mixture of flavors showed good agreement.

**KEYWORDS:** Flavor release; convective mass transfer; volatile permeability; diffusivity; solubility

### INTRODUCTION

Flavor release from foods has been given a lot of importance because it directly reflects consumer satisfaction. Substantial literature is available on the release of different flavor molecules from both model and real food systems either *in vivo* or *in vitro*. The classical works on factors affecting flavor release established the gas–liquid partition coefficient,  $K_{gl}$ , as an important parameter characterizing the affinity of a volatile to the food matrix. Most of the mathematical models including non-thermodynamic approaches developed so far were based on  $K_{gl}$ . Consequently, it is necessary to know this value for each flavor compound for the prediction of its release. However,  $K_{gl}$  values vary with the method used for their determination (1), and methods known for good repeatability are rather time-consuming (1, 2). Katritzsky et al. (3) developed an empirical, quantitative structure–property relationship (QSPR) method that allowed the determination of the effect of salivary components on the partitioning of volatiles (4) and the prediction of the static headspace volatile concentrations above solutions of sucrose (5). McNulty and Karel (6–8) presented ideas on modeling the release process from oil-in-water (O/W) emulsions under nonequilibrium conditions. Darling et al. (9) studied the release of isopentyl acetate from galactomannan and sucrose solutions using the penetration theory. Overbosch et al. (10) reviewed important factors affecting flavor release. The nonequilibrium model developed by de Roos and Wolswinkel (11) focused on the importance of physicochemical parameters of volatiles, such as volatility and hydrophobicity along with the resistance to mass transfer, and studied the effect of ingredients on partitioning from a product phase. Work by Harrison and co-workers resulted in several dynamic release models considering solutions containing aroma-binding macromolecules (12), solid food

matrices (13), gelatin gels (14), and liquid emulsions (15). Effects of a few mouth parameters, such as breathing and saliva flow, were also explained using mathematical correlations (16).

Many of the previous models were developed using theories of interfacial mass transfer, such as the penetration theory, the surface renewal theory, or the boundary layer theory. Conclusive model equations based on diffusion across the interface were developed. They satisfactorily explained the rate-limiting factors for the release process for the matrices studied but often focused on a single flavor compound. Many of the models were not supported by detailed experimentation.

The introduction of APCI-MS techniques into the field by Linforth and Taylor (17) not only facilitated the study of flavor release in real time but also became an ideal tool for the validation of theoretical models. The contribution of Taylor's group was recently reviewed by Linforth (18). Marin et al., for example, developed a mass transfer model combining important physicochemical properties of volatiles and the system environment, which both considerably affect the release process (19, 20). A glass bottle, in which a stream of air diluted the headspace above a stagnant liquid phase, was used for experimental validation. In an extended study by Parker and Marin (21), a new mass transfer cell was developed, which could use both liquid and air in co- or counter-current flow. This cell facilitated a short time contact between air and the liquid phase for the exchange of volatiles, which is close to reality during drinking of beverages.

Recognizing  $K_{gl}$  as the main driver of overall mass transfer, the present study aimed at breaking down this thermodynamic variable into computable variables that appeared to be more appropriate to describe the rapid, presumably nonequilibrium process of *in vivo* flavor release. The novel model was based on convective mass transfer and on some parameters of an apparatus (22) that independently generated experimental data for validation.

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## RESULTS AND DISCUSSION

**Development of the Mathematical Model: General Terms.**

The interfacial mass transfer of volatiles across the interface of pure water and air can be considered to be proportional to the difference in flavor concentration existing in both phases and can be expressed by the relationship

$$V(dC_{hs}/dt) = KA(C_{bp} - C_{hs}) \quad (1)$$

where  $V$  is the volume of headspace ( $hs$ ) in the sample reactor,  $K$  is the mass transfer coefficient, and  $A$  is the surface area of the liquid bulk phase ( $bp$ ) exposed to the air stream in the headspace. Integration of eq 1 within appropriate limits gives the relationship

$$C_{hs}(t) = (1 - \exp^{-(KA/V)t})C_{bp} \quad (2)$$

Equation 2 gives the headspace concentration with respect to time for any flavor compound. The detailed derivation can be found in the Appendix.

**Mass Transfer Coefficient for Forced Convection in a Circular Tube.** When a liquid is under continuous stirring, mass transport is affected by Eddy diffusion (23). In a situation when the headspace is created over a product phase in a very short period of time followed by agitation, the mass transfer coefficient governs the release. Besides the convection process, the physicochemical parameters of the volatiles are directly affecting the partitioning ( $K_{gl}$ ), and the volatility is of crucial importance. We attempted to arrive at a mass transfer correlation sensitive to the minute variations in the physicochemical properties of volatiles and the hydrodynamic parameters of the dynamic release process.

The mass transfer correlation for forced convection in a circular tube under turbulent flow is explained by Cussler (24):

$$K = 0.026(\text{Re})^{0.8}(\text{Sc})^{1/3}(D/l) \quad (3)$$

$\text{Re}$  represents Reynold's number and  $\text{Sc}$  Schmidt's number (see the Appendix). This correlation describes the diffusion of solutes from the wall of a circular tube or a similar process in which solid material diffuses into the liquid phase in turbulent motion.  $D$  represents the diffusivity of the molecule and  $l$  the diameter of the circular tube, which is the radial distance to be traveled by the solute.

**Modified Mass Transfer Coefficient for a Stirred Tank.**

Flavor release depends on the permeation of volatile molecules from the liquid into the headspace. Therefore, eq 3 must be modified (1) for volatile molecules that are unique in their physicochemical characteristics and (2) for the environment in which the release process occurs. Volatiles differ from other molecules mainly in exerting significantly higher vapor pressures, which are in turn affected by the properties of the surrounding medium. Furthermore, when a liquid is under turbulent motion during shear, a volatile molecule is forced to diffuse through the medium itself and, depending on its solubility, purges out into the headspace aided by its volatility. By taking these factors into consideration, a term for volatile permeability ( $P$ ) was obtained, given by the following relationship:

$$P = D \frac{\delta^2}{V_f} \sqrt{\frac{p}{S}} \quad (3a)$$

The permeability of volatile molecules varies directly with the vapor pressure ( $p$ ) and the diffusivity ( $D$ ) and inversely with

**Table 1.** Molecular Weight (MW), Log  $P$ , and Index and Equivalent Numbers of the Volatiles Used for the Calculation of Water Solubility Applying Equation 3b

compound	MW (g mol <sup>-1</sup> )	Log $P$	$N_h$	$N_c$	$N_s$	$N_d$
isobutyl acetate	116	1.71 <sup>a</sup>	1	7	1	1
ethyl 2-methylbutyrate	130	2.26 <sup>a</sup>	1	8	1	1
(Z)-3-hexenyl acetate	142	2.61 <sup>a</sup>	1	6	1	2
2,3-dimethylpyrazine	108	0.64 <sup>b</sup>	0	1	1	2
(Z)-3-hexenol	100	1.61 <sup>a</sup>	1	6	1	3
2-isobutylthiazole	141	2.51 <sup>b</sup>	0	4	1	2
furfuryl acetate	140	1.09 <sup>b</sup>	1	2.5	2	1
linalool	154	3.28 <sup>b</sup>	0	1	1	2
2-pentylpyridine	149	3.32 <sup>a</sup>	0	2.5	0	1
D-carvone	150	3.07 <sup>a</sup>	0	1	0	2
$\beta$ -damascenone	190	4.21 <sup>a</sup>	0	3.5	1	2
diacetyl	86	-1.33 <sup>b</sup>	1	4	1	1

<sup>a</sup> Calculated with SRC's LOGKOW/KOWWIN program (Syracuse Research Corp., <http://esc.syrres.com/interkow/kowdemo.htm>). <sup>b</sup> Calculated with Advanced Chemistry Development (ACD) Software Solaris V 4.67 (1994–2002 ACD).

**Table 2.** Solubility, Diffusivity, and Vapor Pressure Values (at 30 °C) of Flavor Compounds Used in the Study

compound	solubility <sup>a</sup> (kg m <sup>-3</sup> )	vapor pressure <sup>b</sup> (Pa)	diffusivity <sup>c</sup> (m <sup>2</sup> s <sup>-1</sup> )
isobutyl acetate	1.12	2366	1.06E-09
ethyl 2-methylbutyrate	0.31	909	9.83E-10
(Z)-3-hexenyl acetate	0.46	160	9.37E-10
2,3-dimethylpyrazine	260	40	1.09E-09
(Z)-3-hexenol	10.28	95.5	1.13E-09
2-isobutylthiazole	2.8	117	9.57E-10
furfuryl acetate	8.04	106.7	6.87E-10
linalool	0.95	14	8.59E-10
2-pentylpyridine	0.51	28.7	8.58E-10
D-carvone	1.82	6.6	9.37E-10
$\beta$ -damascenone	0.064	10	7.97E-10
diacetyl	1074	6801	1.42E-09

<sup>a</sup> Calculated from eq 3b. <sup>b</sup> Derived from safety data sheets, usually software computed. <sup>c</sup> Reference 25.

the solubility ( $S$ ), as it is an indirect measure of the association parameter of a compound with the water phase. Vapor pressure values were obtained from suppliers' safety data sheets. Such data are usually calculated using advanced software, for example, Advanced Chemistry Development Software Solaris V 4.67 (1994–2002 ACD).  $D$  was calculated by a semiempirical formula suggested by Smith and Harriot (25). The value of  $S$  for all volatile compounds was calculated by a modified log  $P$ -based equation of Meylan et al. (26), as proposed by Larroche and Gros (27)

$$\log(S) = 3.796 - 0.854 \log P - 0.00728(\text{MW}) - 0.537N_h - 0.082N_sN_c + 0.346N_d + 0.310 \quad (3b)$$

where  $N_h$  represents the hydrocarbon index of the molecule, which takes value equal to either 1 or 0 depending on the compound family,  $N_s$  is the saturation index, and  $N_c$  is the carbon number equivalent.  $N_d$  is an integer representing the double-bond equivalent. All of the numbers of each compound together with the molar weight (MW) are given in **Table 1**. The values of  $D$ ,  $p$ , and  $S$  for different aroma compounds are given in **Table 2**. During the flavor release process a laminar flow of air over the bulk phase at a definite flow rate was assumed. Hence, a very thin film of air is in contact with the surface of the bulkphase.  $\delta$  represents this effective film thickness of the headspace (air) in contact with the bulk phase, which plays an important role in the uptake of flavor molecules from the liquid

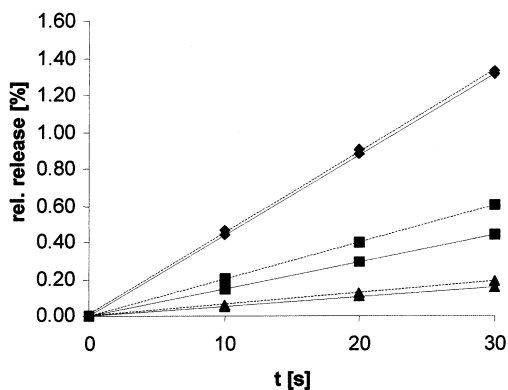


Figure 1. Comparison of model-predicted (solid line) and experimental [dashed line, (22)] pattern of release of (◆) ethyl 2-methylbutyrate, (■) (Z)-3-hexenyl acetate, and (▲) 2-isobutylthiazole.

surface. The value of  $\delta$  is calculated by a mathematical relationship established in the film theory of mass transfer (28). For a given flow rate of air this film thickness remains constant.  $V_f$  represents the volumetric flow rate of air over the bulk phase. It should be noted that an interfacial film of the liquid phase exists at the interface, but this film is considered to be infinitely thin as long as the liquid is well stirred ( $Re \sim 50000$ ) and the observed process time of release is short (30 s).

For the modification of eq 3, the diffusivity  $D$  (which represents the diffusion velocity) of the Sherwood number was replaced by  $P$  and the diameter of the tube  $l$  by  $H_{ln}$ , the logarithmic mean height.  $H_{ln}$  represents the average vertical distance that a flavor molecule has to move in the bulk phase to reach the interface and to be released into the headspace:

$$K = [0.026(Re)^{0.8}(Sc)^{1/3}](P/H_{ln}) \quad (4)$$

With these changes, the mass transfer correlation of eq 4 was used in eq 2 to predict the flavor release.

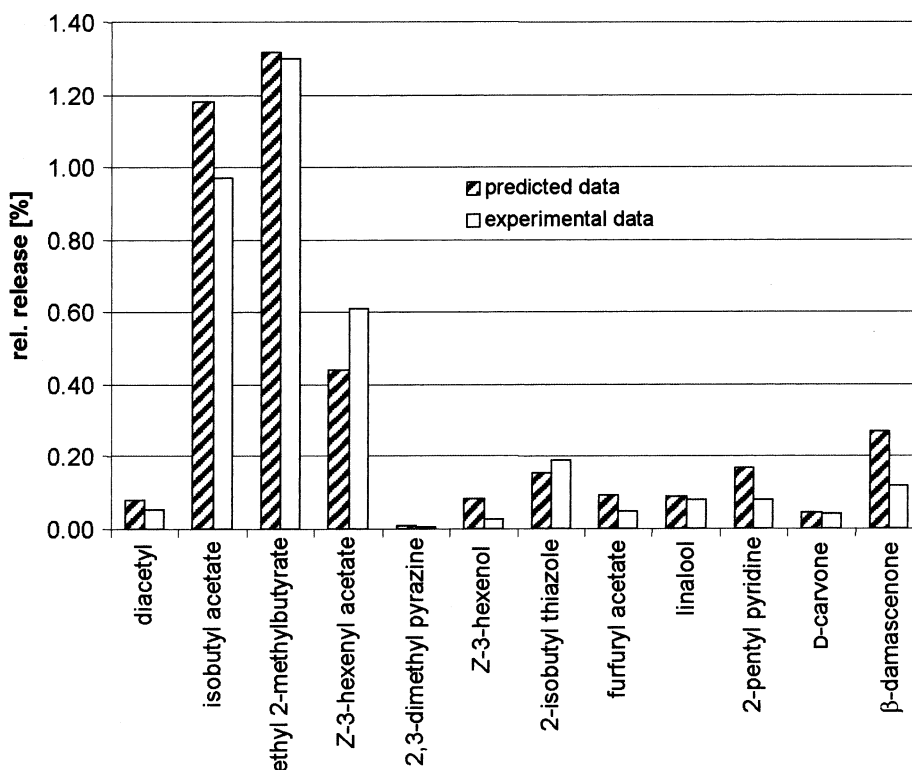


Figure 2. Predicted versus experimental (22) flavor release from water after 30 s.

Table 3. Fixed Process Parameters Applied in the Study Adapted from Reference 22

parameter	setting	parameter	setting
$A$	0.042 m <sup>2</sup>	$\mu$	$7.98 \times 10^{-4}$ kg m <sup>-1</sup> s <sup>-1</sup>
$V$	$8.5 \times 10^{-4}$ m <sup>3</sup>	$\delta$	$1.74 \times 10^{-3}$ m
$V_f$	$1.6 \times 10^{-4}$ m <sup>3</sup> s <sup>-1</sup>	$n$	7.5 s <sup>-1</sup>
$d$	0.07 m	$H_{ln}$	0.15 m
$\rho$	995 kg m <sup>3</sup>		

**Comparison of Model-Predicted and Measured Release Data.** Dynamic flavor release of 12 different flavor compounds from water was predicted using physicochemical data of the volatiles (Table 2) and of water (Table 3) and dimensional and operating parameters (Table 3) of an apparatus previously used to measure dynamic flavor release (22). The model equation (eq 2) predicted a linear correlation between the total flavor quantities released and time (in the first 30 s). Observations of Rabe et al. (22), who reported linear kinetics and coefficients ranging from 0.9911 to 0.9999, matched the model well. A comparison of the predicted and experimental release kinetics for three selected compounds is shown in Figure 1. For periods of time >60 s the model predicts an exponential release profile, with the initial concentration as the rate-limiting factor.

Predicted relative release rates of the flavor molecules at the end of a 30 s period varied from 0.01 to 1.3% depending on their physicochemical properties. Thus, the relative release should differ by a factor of 130 and result in the development of a specific aroma profile in the dynamic headspace. These results of the model are in agreement with data given recently (22) showing that the model is capable of predicting the overall release profile of diverse flavor molecules possessing a wide range of molecular properties. A comparison of the model-predicted and experimental flavor quantities dynamically released after 30 s is shown in Figure 2. The deviations between the predicted and the experimental data were <30% for most of the compounds. The use of improved software for the accurate

calculation of molecular properties of flavor compounds, such as  $p$ ,  $S$ , and  $D$ , might reduce the variation between model-predicted and actual flavor release.

**Usefulness of in Vitro Release Experiments and Modeling.** Studying the factors affecting flavor release in the mouth is a matter of ongoing discussion. Using technical devices the simulation of the human mouth and the complex mechanisms of deglutition is not possible, and only idealized situations of real food consumption can be created (22). Nevertheless, considerable advantages of in vitro approaches, such as their high sensitivity and low variability within experiments, can be used to study release mechanisms, particularly if important mouth conditions have been considered. Further steps are then to model the process of flavor release in these devices and to compare with in vivo data.

The release of volatiles depends on many dimensional and process variables in the mouth. The carry-over of flavor molecules by an air stream from an agitated liquid phase, for example, is highly comparable to mass transfer by forced convection, where the liquid is continuously stirred and an unsaturated stream of pure air with laminar flow, comparable with the situation in the mouth (10), aids in the release of volatiles at the gas-liquid interface. The presented model includes a new mass transfer coefficient (eq 4) for the prediction of dynamic flavor release from pure water. As it was the aim to validate the model with experimental data, a mass transfer coefficient for stirred tanks was applied; previous experiments were conducted using such a device (22). The apparatus simulates important physiological parameters of the mouth cavity, such as temperature, shear rate, saliva addition, and gas flow. These variables (with the exception of saliva addition) were all included in the theoretical model. Saliva was not considered, as it was shown that it had no influence on the release of flavor molecules from liquids in the mouth (29). The temperature of the system, in which volatile release occurs, has a large impact on both the physicochemical properties of the flavor molecules and the hydrodynamic properties of the bulk phase. The model takes this into account, as it predicts the release at an average temperature by incorporating all of the parameters at a particular temperature. The air flow rate is represented in  $P$ , and  $Re$  reflects the shear rate. Therefore, the dynamic nature of both the bulk phase and the headspace are considered.

The model predicts the release of volatiles from water on a time scale, that is, kinetically. The novelty lies in the fact that all of the physicochemical parameters of the model can be theoretically calculated and used for the prediction. The replacement of the sum parameter  $K_{gl}$  by three molecular properties (Table 2) allows the independent consideration of each of these variables. They all address different mechanisms of partitioning and may better account for the fine structure of the flavor molecules. Fixed process parameters (Table 3) translate the convective mass transfer model into the reality of the apparatus used for validation (22). Improved mathematical terms that can better explain the association parameters of flavor molecules with the medium will result in refined model versions. A deeper insight into the molecular properties of flavor molecules, their changes caused by the physical environment, and physicochemical interactions with food components might lead to extended versions of models for a variety of food matrices.

#### ABBREVIATIONS USED

$V$ , volume of the headspace ( $m^3$ );  $C_{hs}(t)$ , volatile concentration in the headspace at any time  $t$ ;  $K$ , mass transfer coefficient ( $m$

$s^{-1}$ );  $A$ , interfacial area ( $m^2$ );  $t$ , time (s);  $C_{bp}$ , initial volatile concentration in the bulk phase;  $Re$ , Reynold's number;  $d$ , diameter of the stirrer (m);  $\rho$ , density of the bulk phase ( $kg\ m^{-3}$ );  $\mu$ , viscosity of the bulk phase ( $kg\ m^{-1}\ s^{-1}$ );  $n$ , number of rotations of the stirrer ( $s^{-1}$ );  $Sc$ , Schmidt's number;  $D$ , diffusivity ( $m^2\ s^{-1}$ );  $l$ , diameter of the circular tube (m);  $P$ , volatile permeability ( $m^2\ s^{-1}$ );  $\delta$ , effective film thickness of flowing air in contact with the bulk phase (m);  $V_f$ , volumetric flow rate of air ( $m^3\ s^{-1}$ );  $p$ , vapor pressure (Pa);  $S$ , aqueous solubility ( $kg\ m^{-3}$ );  $MW$ , molar weight ( $g\ mol^{-1}$ );  $N_h$ , hydrocarbon index;  $N_s$ , saturation index;  $N_c$ , carbon number equivalent;  $N_d$ , double-bond equivalent;  $H_{ln}$ , logarithmic vertical distance in the reactor (m).

#### APPENDIX: MODEL FOR FLAVOR RELEASE BASED ON CONVECTIVE MASS TRANSFER

Mass balance is given by

$$V(dC_{hs}/dt) = KA(C_{bp} - C_{hs})$$

where  $K$  is the mass transfer coefficient and  $C_{hs}(t = 0) = 0$ .

Integrating between the limits

$$\int_0^{C_{hs}} \frac{dC_{hs}}{C_{bp} - C_{hs}} = K \frac{A}{V} \int_0^t dt$$

$$\ln \frac{(C_{bp} - C_{hs})}{C_{bp}} = - \frac{KA}{V} t$$

$$C_{bp} - C_{hs} = C_{bp} \exp^{-(KA/V)t}$$

$$C_{hs}(t) = (1 - \exp^{-(KA/V)t})C_{bp}$$

Dimensionless numbers used in the model are

$$Sc = \text{Schmidt's number} = \mu/\rho D$$

$$Re = \text{Reynold's number} = d^2 n \rho / \mu$$

and

$$Sh = \text{Sherwood's number} = KI/D$$

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