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Calculation of vapor pressure curves for hydroxy benzoic acid derivatives using thermogravimetry

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Abstract

This study aims at providing a simple thermogravimetric method in estimating the vapor pressure characteristics using the Antoine equation as the analytical tool. The heat treatment for the majority of benzoic acid derivatives follows zero order rate processes that are in good correlation with their evaporation process. The optimum conditions for the rising temperature experiments were found when the heating rate was 10 °C/min in an atmosphere of dry nitrogen (100 ml/min). Methyl paraben was taken as the calibration compound since its Antoine constants are reported in literature and its selected thermodynamic parameters were evaluated using the Langmuir equation. The coefficient of vaporization k was determined to be 124525 ± 0.8, with units being reported in the SI system. The corresponding vapor pressure plots were obtained for the remaining compounds that followed a zero order evaporation process and their Antoine constants were calculated using the Levenberg–Marquardt least square curve fit method.

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Keywords: Thermogravimetry; Antoine; Langmuir; Vapor pressure; Benzoic acids

1. Introduction

Benzoic acid derivatives find wide application in the pharmaceutical, chemical and food industry. *ortho*-Hydroxy benzoic acid, commonly known as salicylic acid, is a pharmaceutically active antipyretic agent and *para*-hydroxy benzoic acid and its derivatives form the majority of the pharmaceutical analgesics and antipyretic agents. Chemically, they also are the parent compounds to most of the preservatives that are in use in the food industry. Chemical characterization of these compounds is necessary to predict their behavioral patterns during manufacturing and other industrial processes. The purpose of this study is to look into the effects of those heat treatments on these compounds. The variability in the effects can be determined by performing the calculations for the kinetics of their decomposition, and second, by applying suitable evaporation methodology in order to evaluate the vaporization characteristics for the compounds. The kinetics of evaporation and/or decomposition has to be applied as and when necessary.

Evaporation can be stated to be the transition from the liquid phase to the vapor phase, without a change in chemical composition. Factors such as vapor pressure of the substance, molecular weight, amount of exposed surface area, etc. can alter the evaporation patterns. The primary influencing factor, however, is the rising temperature conditions that the preservatives are being subjected to. The evaporation parameters can

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be determined by the rate of mass loss as the substance undergoes the phase transition from liquid to vapor. This can be achieved with a rising temperature program in thermogravimetric analysis.

A decomposition reaction is defined as a chemical process in which a chemical is degraded into a simpler species. Such reactions include processes in which the crystal lattice structure is destroyed, such as melting, evaporation, sublimation, as well as chemical reactions that result in the formation of a new compound [1]. In all solid-state decompositions, the transformation occurs in an area of enhanced activity, referred to as the reaction interface or the boundary between the reactant and the product [1]. The decomposition of substances can be described on the basis of chemical kinetic principles. Such kinetics are described as zero order, first order or pseudo first order reactions. In solid-state reactions, contrary to conventional chemical kinetic studies, the concentration is not monitored, because it does not vary in a manner that can be correlated with changes in the quantity of the remaining reactant [1]. The fraction reacted α is a better measure for performing the calculations in such reactions.

1.1. Evaluation of kinetics

As a substance undergoes phase transition from liquid to vapor, determining the rate of mass loss can monitor the evaporation process. This is achieved by thermogravimetry, using a linear rising temperature program [2]. The TGA curve that shows a plot of mass against temperature or time is converted into a DTG curve, which measures the rate of mass loss ($\mathrm{d}m/\mathrm{d}t$) against temperature. The shape of the DTG plot, then, would be instrumental in assigning a preliminary kinetic mechanism to the process. In the case of an ideal zero order mechanism, the DTG plot shows a maximum value for ($\mathrm{d}m/\mathrm{d}t$) at a point where all the material is exhausted, so the return of the DTG curve to the baseline is very abrupt and perpendicular in nature. The fraction evaporated (α) is calculated using the following equation:

$$\alpha = \frac{m_\mathrm{i} - m_\mathrm{t}}{m_\mathrm{i} - m_\mathrm{f}} \qquad (1)$$

where m_i and m_f are the initial and final masses in milligrams, respectively [2]. The mass at the specific time is represented as m_t. The data points are obtained from the rising portion of the DTG plot [3]. If a plot of α versus time or temperature were constructed, a sigmoidal shaped curve would be obtained. If evaporation occurs, the fraction evaporated would be obtained as the product of the time and the coefficient of evaporation (k_vap), which can be represented as follows:

$$\alpha = k_\mathrm{vap} t \qquad (2)$$

At constant temperature, k is equal to $\mathrm{d}\alpha/\mathrm{d}t$ [3]. The rate of evaporation is represented by $\mathrm{d}m/\mathrm{d}t$. For zero order rate processes, the coefficient of evaporation can be calculated by dividing $\mathrm{d}m/\mathrm{d}t$ by the cross-sectional area of the crucible used for the sample. In the present study, the evaporation takes place from the liquid interface for two of the three compounds studied. When $\ln k_\mathrm{vap}$ is plotted against $1/T$, a straight line is obtained, with a slope equal to E_vap/R, where E_vap is the activation energy of evaporation and R the universal gas constant. Such plots are consistent with the Arrhenius equation

$$k_\mathrm{vap} = A\,\mathrm{e}^{-E_\mathrm{vap}/RT} \qquad (3)$$

or

$$\ln k_\mathrm{vap} = \ln A_\mathrm{vap} - \frac{E_\mathrm{vap}}{RT} \qquad (4)$$

where A_vap is the pre-exponential factor. For other decomposition mechanisms, the results can be correlated to a set of models, which are based on nucleation, diffusion, reaction order or geometrical factors of the reactant–product interface [4]. The reaction rate in solid-state decomposition is given by

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = kf(\alpha) \qquad (5)$$

where $f(\alpha)$ is a function of α and t the time [5]. This can be made to relate to the temperature by

$$\frac{\mathrm{d}\alpha}{\mathrm{d}T} = \left(\frac{\mathrm{d}\alpha}{\mathrm{d}t}\right)\left(\frac{\mathrm{d}t}{\mathrm{d}T}\right) = \frac{kf(\alpha)}{\beta} \qquad (6)$$

where β is the heating rate ($^\circ\,\mathrm{s}^{-1}$) [6]. This equation can be transformed to the form

$$k = \frac{(\mathrm{d}\alpha/\mathrm{d}T)\beta}{f(\alpha)} \qquad (7)$$

The term $f(\alpha)$ can be obtained from the tables of different mechanisms. For zero order, it is equal to

Table 1
Solid-state rate expressions for deceleratory α-time curves

$g(\alpha) = kt$		$f(\alpha) = (1/k)(\mathrm{d}\alpha/\mathrm{d}t)$
Geometrical models		
R2	$1-(1-\alpha)^{1/2}$	$2(1-\alpha)^{1/2}$
R3	$1-(1-\alpha)^{1/3}$	$3(1-\alpha)^{2/3}$
Diffusion mechanisms		
D1	α^2	$(1/2)\alpha$
D2	$(1-\alpha)\ln(1-\alpha)+\alpha$	$[-\ln(1-\alpha)]^{-1}$
D3	$[1-(1-\alpha)^{1/3}]^2$	$3/2(1-\alpha)^{2/3}[1-(1-\alpha)^{1/3})^{-1}$
D4	$(1-2\alpha/3)-(1-\alpha)^{2/3}$	$3/2[(1-\alpha)^{-1/3}-1]^{-1}$
Reaction order		
F1	$-\ln(1-\alpha)$	$1-\alpha$
F2	$(1-\alpha)^{-1}$	$(1-\alpha)^2$
F3	$(1-\alpha)^{-2}$	$(1/2)(1-\alpha)^3$

one, and for first order, it is equal to $(1-\alpha)$ [5]. Using the Arrhenius method

$$\ln\left[\frac{(\mathrm{d}\alpha/\mathrm{d}T)\beta}{f(\alpha)}\right] = \ln A - \frac{E}{RT} \tag{8}$$

A plot of $\ln[(\mathrm{d}\alpha/\mathrm{d}T)\beta/f(\alpha)]$ versus $1/T$ can be utilized to determine the Arrhenius parameters. A summary of various $f(\alpha)$ expressions can be obtained from Table 1 [4].

1.2. The Antoine equation

In a moderate pressure range, the Antoine equation is an excellent empirical tool, primarily used for curve fitting purpose [7]. It can be written as

$$\ln P = a - \frac{b}{T+c} \tag{9}$$

where P is the vapor pressure, T the absolute temperature, $a = 2.303A$, $b = 2.303B$, and $c = C$. Here A, B, and C are the Antoine constants at a given temperature range, obtained from the book by Stephenson and Malanowski [8]. It is mainly used to evaluate the temperature dependence of vapor pressure. The Antoine constants have been recorded for methyl paraben and the values are: $A = 5.23662$, $B = 1159.34$ and $C = -220.03$, for a given temperature range of 446–517 K. The value of P was obtained at each temperature point from 446 to 501 K, the temperature range being decided upon from the rising portion of the DTG curve.

1.3. The Langmuir equation

The Langmuir equation can explain the evaporation phenomenon

$$\frac{\mathrm{d}m}{\mathrm{d}t} = P\alpha\left(\frac{M}{2\pi RT}\right)^{1/2} \tag{10}$$

where $\mathrm{d}m/\mathrm{d}t$ is the rate of mass loss per unit area, P the pressure, α the vaporization constant, T the absolute temperature, R the universal gas constant and M the molecular weight of the evaporating vapor. The objective is to find out the vaporization constant in presence of a purge gas [9].

Langmuir spent considerable time discussing the value of the vaporization constant and was of the opinion that it is unity if the initial conditions were those of a vacuum but did not exclude the fact that it may have different values from unity. For the use of the Langmuir equation for the TG data, one must assume the fact that α is a constant that is not unity in the presence of a purge gas. The Langmuir equation holds true for a certain rate of mass loss in volatilization from a given container exposing a constant area of interface. It depends a lot on the experimental set up and is independent of the vapor being examined, provided it is not associated.

Eq. (10) can be rewritten as

$$P = [\alpha^{-1}(2\pi R)^{1/2}]\left[\left(\frac{T}{M}\right)^{1/2}\left(\frac{\mathrm{d}m}{\mathrm{d}t}\right)\right] = kv \tag{11}$$

where $k = \alpha^{-1}(2\pi R)^{1/2}$ and $v = (T/M)^{1/2}(\mathrm{d}m/\mathrm{d}t)$.

Since v would be a constant for a given set of experiments, the plot of P versus v would give the value of k. Alternatively, if we take the logarithm of the above equation, then a plot of $\log P$ versus $\log v$ would give the value of $\log k$ [10].

In the set of experiments performed, the instrument was calibrated with methyl paraben as the standard, which gave the value of k. The pressure versus temperature plot was performed. This coefficient of vaporization value thus obtained would be theoretically constant and independent of the substance used. This value was taken for *ortho*- and *meta*-hydroxy benzoic acids. Eq. (11) could be effectively utilized for each substance as the v-value for each substance would be a constant and substituting the k-value will give the corresponding pressure values at each temperature. The vapor pressure plots were then obtained from the data.

1.4. The Clausius Clapeyron equation

The enthalpy of vaporization (ΔH_{vap}) can be calculated for each of the compounds from the Clausius Clapeyron equation, the final form of which is as follows:

$$\log\left(\frac{p_2}{p_1}\right) = \left[\frac{\Delta H_{\mathrm{vap}}}{2.303R}\right]\left[\frac{T_2 - T_1}{T_1 T_2}\right] \qquad (12)$$

where p_2 and p_1 are the corresponding vapor pressures at temperatures T_2 and T_1, respectively, and R the universal gas constant.

1.5. Curve fitting for Antoine constants

Non-linear regression analysis is a useful tool for curve fitting purposes. The empirical Antoine constants for each compound can be effectively determined by the “least square curve-fit” method where the vapor pressure plot for each compound is fitted to the Antoine equation. The parameters A, B, and C would be susceptible to changes depending on the algorithm used. For practical purposes, the Levenberg–Marquardt algorithm [11] was used and the “global” least square fit was found to be consistently accurate in predicting the Antoine parameters. The two most important considerations during such curve fitting operations are as follows:

1. The method of statistical iterations can be easily subjected to change according to the stipulations (or constraints) applied by the experimenter [11]. Thus, after the meeting of the convergence criteria in non-linear regression iterations, it is mandatory to use the values for A–C and corroborate the fact that these parameters indeed describe the vapor pressure curve.
2. All statistical software used for non-linear regression purposes requires a starting value for each parameter before it proceeds with the iterations. This task might be simplified if the Antoine values for one of the compounds in the homologous series being evaluated are known. It can be expected that the unknown Antoine parameters for the compounds in study will not differ by a very large extent compared to the one in its homologous series. For the present study, the starting values stipulated in ASTM methods E1719 and E1782 have been used.

2. Experimental

2.1. Materials

Methyl paraben (laboratory grade) was obtained from Fisher Scientific Company (lot number 762258); ethyl paraben was obtained from Ruger Chemical Company (lot number 1656K); propyl paraben was obtained from Sigma Chemical Company (lot number 31F0416); butyl paraben was obtained from Sigma Chemical Company (lot number 128F0389); salicylic acid was obtained from Sigma Chemical (lot number 52H3418); *meta*-hydroxy benzoic acid was obtained from Sigma Chemical (lot number 33H7709); and *para*-hydroxy benzoic acid was obtained from Sigma Chemical (lot number 121H0539). Their purity grades were stipulated according to USP specifications and were used as received.

2.2. Equipment

The SDT 2960 simultaneous TGA–DTA, from TA instruments, with Thermal analyst 2000 TA operating system version 1.0 was employed to investigate the evaporation behavior of the parabens. An electronic flow meter from J&W Scientific, model ADM 1000 was used to regulate the flow of dry nitrogen (purge gas) through the samples. The SPSS 10.0 software was used to perform non-linear regression analysis.

2.3. Procedure

Rising temperature experiments were performed on the sample and readings were taken at every 1 °C to give accuracy to the results. The runs were conducted in a temperature range from ambient to 400 °C. The heating rate was fixed at 10 °C/min. Nitrogen was used as the purge gas and its flow rate was fixed at 100 ml/min. An open, 110 μl platinum crucible with a cross-sectional area of 0.34 cm^2, was used to contain the sample and an empty platinum crucible of equivalent area was used as the reference. The sample size was chosen so as to cover the base of the crucibles uniformly and to about one-third of its capacity.

Data from the DTG plot on methyl paraben was first used to construct the Arrhenius plot from which the activation energy was obtained. From the Clausius Clapeyron plot for methyl paraben, the latent heat of evaporation was obtained. The Antoine and Langmuir equations were then used to obtain the coefficient of evaporation k, from which the vapor pressure curve was constructed. The Antoine constants were reported in the literature and were as follows: $A = 5.23$, $B = 1159.34$, and $C = -220.03$, for a temperature range of 446–499 K. Calculations for the kinetics were performed and the decomposition for all the compounds studied were determined to be zero order in nature, except for *para*-hydroxy benzoic acid. *para*-Hydroxy benzoic acid followed a first order mechanism and therefore, was not subjected to evaporation kinetics. The vapor pressure curves for *ortho*- and *meta*-hydroxy benzoic acids were constructed by taking into account the k-value obtained from methyl paraben, as the coefficient of evaporation is independent of the sample.

3. Results and discussion

3.1. Calculations for kinetics

From the TG–DTG curves of the methyl paraben (Fig. 1), ethyl, propyl and butyl parabens (Fig. 2), and *ortho*-, *meta*- and *para*-hydroxy benzoic acids (Fig. 3), the rising portions of the DTG curves were taken and the kinetics were determined. The Arrhenius equation parameters are tabulated in Table 2. All compounds except for *para*-hydroxy benzoic acid follow zero order kinetics, which are non-activated processes.

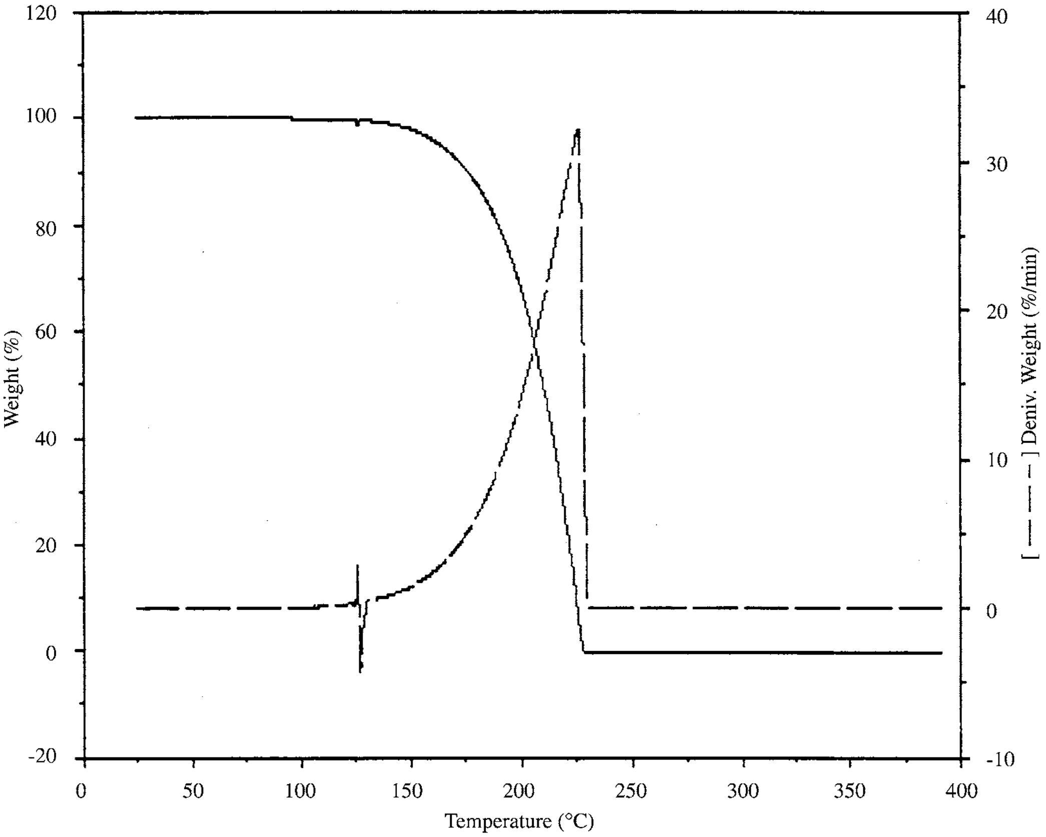

Fig. 1. TG–DTG plot for methyl paraben.

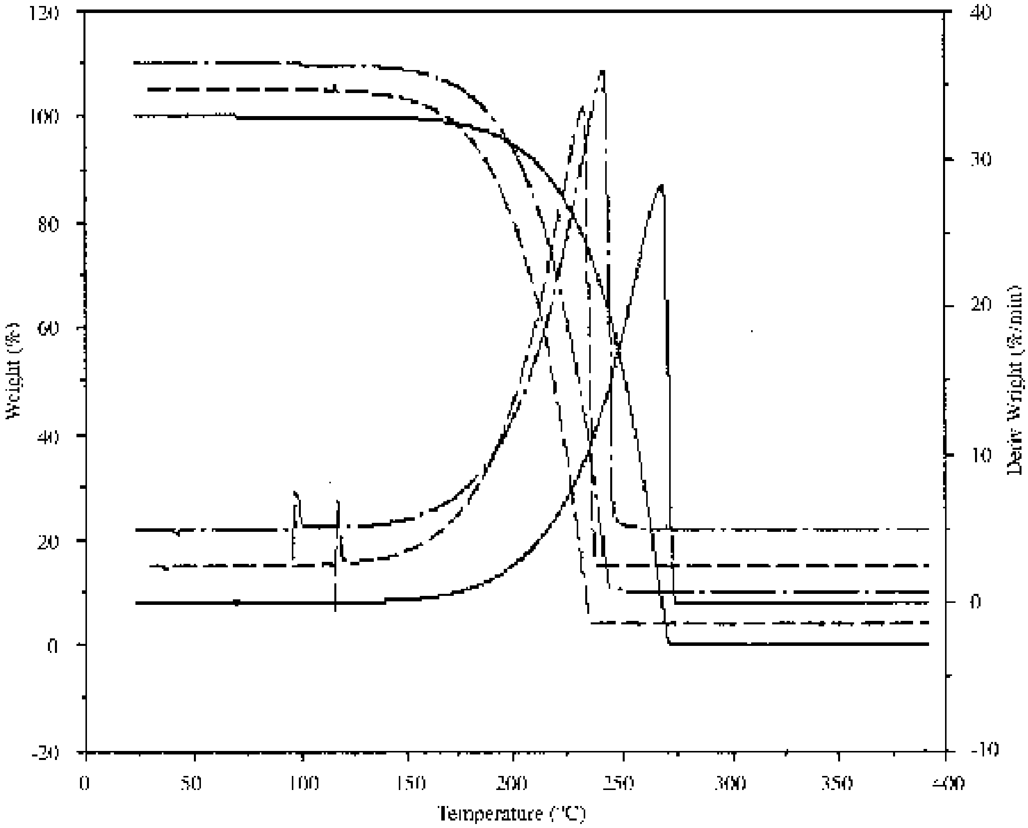

Fig. 2. TG–DTG plots for ethyl (- - -), propyl (– · – · –) and butyl (—) parabens.

Their latent heats of evaporation values closely correspond to their energy of activation values as is evident from the ΔH_{vap}, values obtained (Table 2). For *ortho*-hydroxy benzoic acid, intramolecular hydrogen bonding is observed and there is no association between two adjacent molecules. Thus, a zero order evaporation process is observed. For the *para*-derivative, intermolecular hydrogen bonding is observed that result in an association between adjacent molecules [12]. Greater thermal energy is needed to break such hydrogen bonding and thus a zero order evaporation process is not observed. The energy of activation for *para*-hydroxy benzoic acid is 119.1 kJ mol^{-1}, which is far greater than 64.8 and 78.2 kJ mol^{-1} for the *ortho*- and *meta*-derivatives, respectively. Thus, the decomposition of *para*-hydroxy benzoic acid is not a non-activated

Table 2
Arrhenius equation parameters and latent heats of vaporization for the compounds studied

Compound	E_{act} (kJ mol^{-1})	ln A	R^2	ΔH_{vap} (kJ mol^{-1})
Methyl paraben	70.3	15.9	0.998	77.1
Ethyl paraben	73.1	16.3	0.998	75.0
Propyl paraben	77.1	16.9	0.999	79.1
Butyl paraben	74.8	15.4	0.995	76.9
Salicylic acid	64.8	15.3	0.997	66.7
meta-Hydroxy benzoic acid	78.2	16.3	0.996	80.1
para-Hydroxy benzoic acid	119.1	26.1	0.997	–

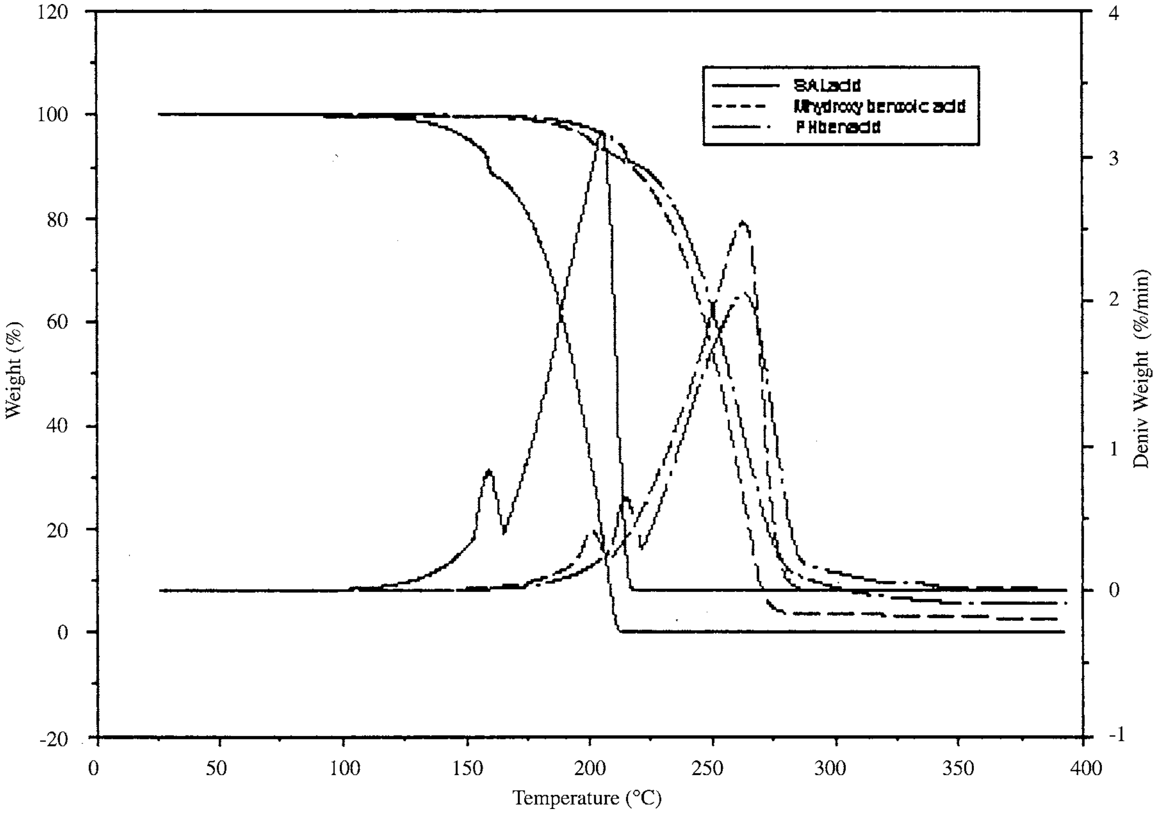

Fig. 3. TG–DTG plots for salicylic (—), *meta*-hydroxy benzoic (- - -) and *para*-hydroxy benzoic (– · – · –) acids.

process and requires considerably more thermal energy than its homologues to undergo decomposition. No such complications are observed for the paraben series, as all are quite susceptible to evaporation processes.

3.2. Vapor pressure calculations

Methyl paraben was taken as the calibration compound and a plot of log P against log v (Fig. 4) was used to obtain the value of k from the Langmuir equation. The coefficient of evaporation k obtained from methyl paraben was determined to be 124525 ± 0.8, units being in the SI system. The vapor pressure curve for methyl paraben was constructed from the Antoine constants reported in the literature and is seen in Fig. 5. Using the derived method of indirectly using the k-value, the vapor pressure curves for the other compounds were constructed (Fig. 6).

Non-linear regression was used to calculate Antoine constants for each of the six compounds. The starting values for the constants A, B, and C were 9.3, 2000 and -37, respectively, the values being valid for pressure in Pascals and temperature in Kelvin. Constructing the theoretical vapor pressure curves and comparing them with those calculated validated the parameters obtained. Acceptable agreement was obtained proving the Levenberg–Marquardt algorithm [11] utilized for the process is adequate. The Antoine constants are given in Table 3.

3.3. The value of *k*

The coefficient of vaporization k is perhaps the most important parameter in the Langmuir equation that is being utilized in such studies. This parameter is a constant, and is independent of the material being studied. In a recent study Price and Hawkins [13] have

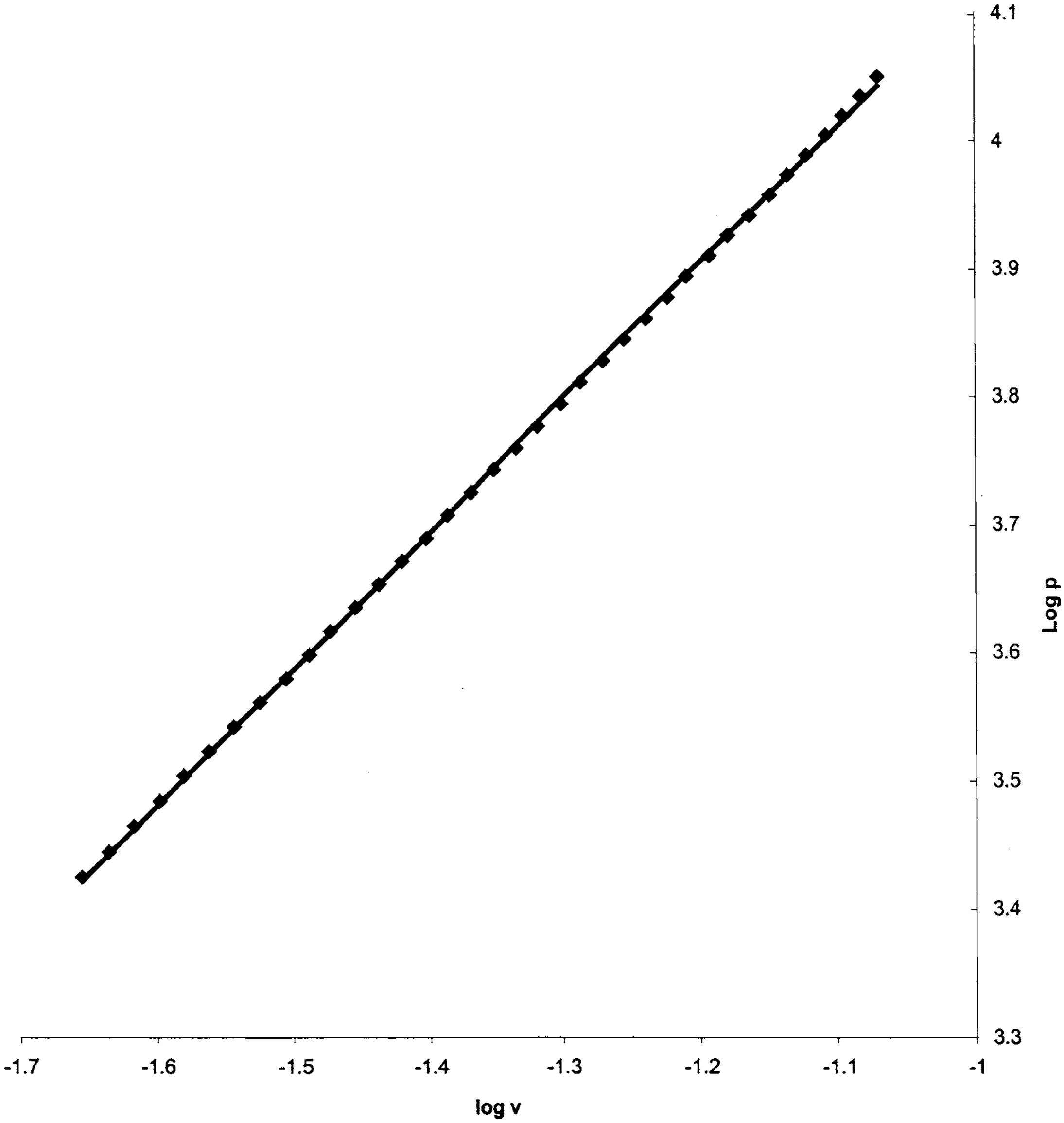

Fig. 4. Calculation for k; plot of log P against log v.

reported the value of k in the CGS system of units. In this study, it was deemed best to use SI units in a uniform manner and the value for k was found to be 124525 ± 0.8. This is in good correlation with the reported value of k in the literature. This study confirms that it is prudent to keep the units in the SI system and thus the value of k is in the vicinity of 1.2×10^5.

3.4. Value of α

Langmuir had theoretized that the value of α should be unity [9]. However, he did not exclude the possibility that it could have other values as well. An interesting feature of this study is that the conversion of all the units to the SI system gives a considerably large k-value that makes the α-value small. Moreover,

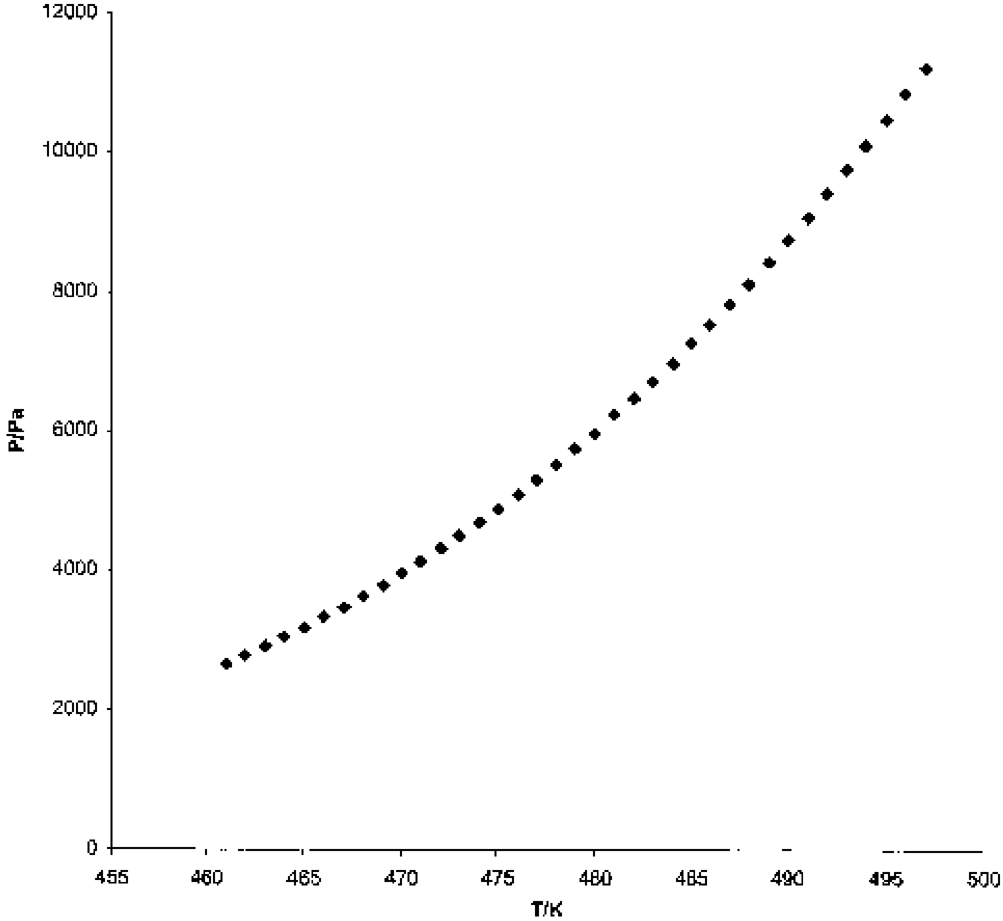

Fig. 5. Vapor pressure plot for methyl paraben.

the value of unity for α might hold true in a vacuum, but in the presence of a purge gas, it might change considerably. In this case the purge gas was dry nitrogen. This constant might be useful in calculating the vapor pressure of related substances as well since it assumes the independence of the material used provided that there is no inter-nor-intramolecular association. Going by the Langmuir equation, the *k*-value

Table 3
Antoine constants for the compounds undergoing evaporation

Compound	Antoine constants			Temperature range (K)
	A	*B*	*C*	
Methyl paraben[a]	5.23	1159.34	220.03	446–499
Ethyl paraben	7.32	794.37	−260.86	448–505
Propyl paraben	8.66	1491.58	−190.66	448–510
Butyl paraben	6.32	357.52	−363.96	498–542
Salicylic acid	6.28	316.74	−319.88	441–477
meta-Hydroxy benzoic acid	6.35	374.47	−360.21	493–537

[a] Antoine constants are reported in the literature.

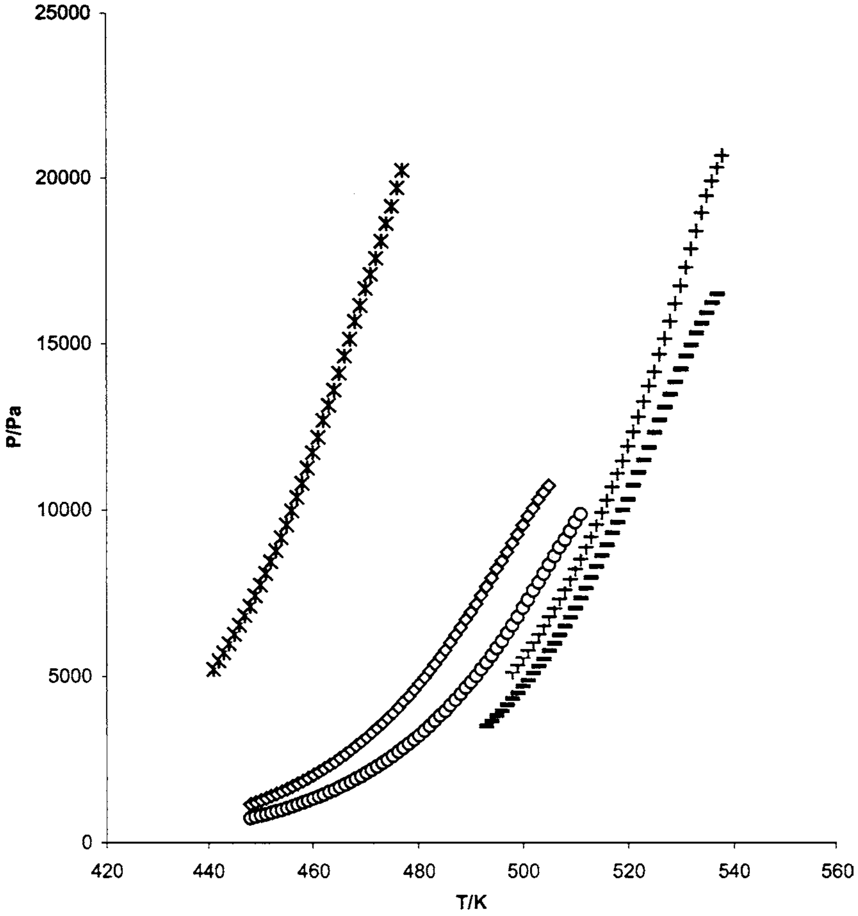

Fig. 6. Vapor pressure plot for ethyl paraben (◇), propyl paraben (○), butyl paraben (+), salicylic acid (×), and *meta*-hydroxy benzoic acid (–).

is inversely proportional to α. Langmuir had opined that the value of α is unity under vacuum conditions [9], though he did not categorically state that it cannot change under the influence of a purge gas. It is important to note that the experimental design utilized in this study would have a multicomponent atmosphere. First, there is nitrogen as the purge gas and second, the compound being investigated is itself vaporizing and continuously adding to the partial pressure of the material. This expectedly would alter the value for α. However, the value of α is obtained as 5.8×10^{-5}. This extremely small quantity cannot be explained yet with the resources currently available. Further research should be performed in this direction to critically evaluate the value of α.

3.5. *Clausius Clapeyron plots*

Clausius Clapeyron plots were generated for each compound in the study. Such plots have log P (logarithm of pressure) in the Y-axis and the reciprocal of absolute temperature $1/T$ in the X-axis. Those compounds, which exhibited zero order evaporation processes were taken into consideration and their Clausius Clapeyron plots were generated, the equations of which are tabulated in Table 2. An obvious anomaly was observed in a few of the plots. The plots generated a curve rather than a straight line. If the plot is curvilinear in nature, fitting a straight line for regression parameters is futile. For the regression parameters and R^2-value to have any significance, the points must be perfectly scattered in nature. Ethyl paraben, butyl paraben, and salicylic acid, have very pronounced curvilinear trends. This suggests that the Clausius Clapeyron equation will not be ideal in constructing vapor pressure plots, since it is not always obeying the basic assumption of any statistical operation, which presupposes the random scatter of points. It is imperative, therefore, that the Antoine equation has a better physical and statistical significance when vapor pressure curves are to be constructed.

3.6. Starting parameters for iterations

In order to compute iterations for non-linear regression, one has to specify the starting parameters for the Antoine constants. This might not be always an easy task. ASTM methods E1719 and E1782 specify the starting values for A, B and C to be 9.3, 2000 and -37, respectively, when the pressure is in Pascals and temperature is in Kelvin [14]. For the list of compounds studied, these values proved to be useful as they generated acceptable curve fits. If these values did not prove to be useful, one had to take into consideration a different algorithm in order to arrive at acceptable curve fits. Operating with the same parameter constraints would be valid only if the compounds under study are chemically similar in nature. Two compounds having totally different chemical entities might not follow the same analogies when their vapor pressure curves are being verified for suitable curve fits.

4. Conclusions

This work demonstrates a comprehensive technique in characterizing chemical moieties by rising temperature thermogravimetric analyses. This work also suggests that thermogravimetry is an effective technique for the determination of the coefficient of vaporization, when the Antoine vapor pressure constants and the molecular weights of the substance in the vapor phase are known. Linear rising temperature conditions are very useful in obtaining a rapid means of measurement. For substances whose Antoine constants are not reported, a known substance can be effectively used to calibrate the procedure and the vapor pressure curve for that unknown substance can be plotted. The statistical procedure of non-linear regression analysis by the global least square fit method, can be effectively used to calculate the unknown Antoine parameters. There might be some disagreement regarding the value of α, since from this study its value was determined to be extremely small. However, this method can be effectively utilized as a rapid and reliable means of estimating the vaporization characteristics for pharmaceutical and in general, chemical ingredients.

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