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Engineering investigations of the vapour-liquid-equilibrium of flavour-components at atmospheric wort boiling conditions (98.1 – 99.0 °C)

An important function of the boiling of wort is the evaporation of unwanted flavours. If the over-all evaporation is not sufficient, off-flavour will occur in beer. Furthermore, a decrease in the flavour stability can be recognised. The needed total evaporation to undershoot a required concentration of a flavour component at a given primary concentration in wort is given by the vapour-liquid-equilibrium (VLE) of the component and wort, respectively water. If the VLE of a flavour component is known, it is possible to calculate residue curves. In the case of wort boiling, these residue curves give a relationship between the percentage decrease of a flavour and the percentage evaporation of wort. Because of this, it is possible to calculate a needed over-all evaporation if the VLE, the required concentration of a compound at the end of boiling, and the primary concentration of the compound in the kettle up wort are known. For this, the VLE-diagrams of the most important flavours in pure water were acquired in this work. In contrary to the boiling of a mixture of flavour compounds in pure water, where no recreation takes place, it is in the case of boiling wort also necessary to know the recreation of the considered flavour compounds. Because of this, the rate constants of the same compounds that were investigated in this work, were measured in a former article. The recreation of a flavour depends only on the boiling temperature and boiling time. Thus, the results of the former article can be combined with the results of this article in terms of residue curves, if the evaporation rate is known. This calculation will be given in a follow up article in this journal.

Descriptors: Wort boiling, vapour-liquid-equilibrium, flavour-components, flavour stability

1 Introduction

An important function of the boiling of wort is the evaporation of unwanted flavours. If the total evaporation is not sufficient, off-flavour will occur in beer. Furthermore there is a decrease in the flavour stability. The aim of this work is to get cognition of the steaming behaviour of important flavours that have to be reduced during the boiling of wort.

The liquid part of wort consists mainly of water with flavour components in high dilution. For this, the vapour-liquid-equilibrium (VLE) was acquired for wort flavour components in pure water at high dilution. With the knowledge of the VLE, residue curves for atmospheric boiling conditions can be calculated to predict a needed total evaporation individually for every brew. In opposite to residue curves of flavour-components in pure water, in which no recreation takes place, a possible recreation of compounds during wort boiling must be considered in the calculation of these curves in wort. For this, the rate constants of the same compounds investigated herein were measured in a former work [1]. The typical odour impressions of the investigated compounds were also cited in the former work. The recreation of a flavour depends only on the boiling temperature and boiling time [2, 3]. Thus the results of the former article can be combined with the results of this work in terms of residue curves, if the evaporation rate is known.

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Tables and figures see Appendix

The needed total evaporation to undershoot a required concentration at a given primary concentration in wort is a property of the solution and cannot be affected by atmospheric wort boiling systems, although this is often claimed [4-8]. It can only be increased by a flash evaporation [9].

The VLE of components in such a high dilution, such as flavour components in wort are situated, is given by the limiting separation factor of a component in water. Limiting separation factors (K_i^∞) are measures of the VLE behaviour of highly dilute solutions. One technique to determine K_i^∞-values is the measurement of vapour and liquid equilibrium compositions of highly dilute mixtures sampled from a recirculating still [10]. This method provides a simple and direct experimental technique, if an accurate method for the analysis of the liquid and condensed vapour samples is available. Since the absorption of UV light by phenylethanal, 2-phenylethanol, 2-furfural, γ-nonalactone and benzaldehyde is very strong, UV spectroscopy provides such an accurate method. As the absorption of UV light of the other investigated components (dimethylsulfide (DMS), 2-methylbutanal, 3-methylbutanal and hexanal) is very low, gas chromatographic (GC) analysis had to be applied. All measurements were performed at atmospheric boiling conditions (946 – 977 mbar; boiling point: 98.1 – 99.0 °C). To figure out if the limiting separation factors differ to those at constant ambient condition of 1013 mbar (boiling point: 100 °C), the results were combined with literature data, when these were available. This procedure occurred to figure out whether the location of a brew house (different ambient conditions / different boiling points of wort) has an influence on the VLE of flavours during atmospheric boiling of wort.

2 Fundamentals

The VLE of flavours in wort

As this work focuses only on the VLE of highly diluted components, no explanation of the thermodynamic fundamentals of the VLE

behaviour in less dilute mixtures is given. A detailed description of these fundamentals can be found elsewhere [11-13]. Furthermore, the fundamentals of the VLE in highly diluted solutions given in this article were simplified to the extend that is needed to understand the behaviour of flavours during the boiling of wort. A detailed description of the VLE behaviour of highly diluted components can be found in the literature [14, 15].

The VLE of a flavour compound highly diluted in wort is given by the limiting separation factor of the component in water. At conditions with a mole fraction x_i of a component $i \leq 10^{-6}$, the state of dilution is called infinite dilution. As the mole fraction of flavour components in wort is clearly less ($x_i \leq 10^{-8}$), all components lie in the limit of the infinite dilution, and each flavour molecule (solute) in wort is only surrounded by water (solvent) molecules, whereupon only solute-solvent interactions can occur. Thus, the VLE of each compound in wort can be regarded as a two substance VLE between water and the aromatic compound [14].

However, wort is not only a mixture of water and flavours. Aboundingly present, there is also the original wort (gravity), which is the sum of all soluble, non volatile components [16]. This original wort consists mainly of different sugars and proteins, which could influence the thermo-dynamic behaviour of flavours in comparison to their behaviour in pure water. Carbohydrates in high amounts (≥ 25 - 30 %) can affect the VLE of flavours in a form that can be compared to a salting-out-effect [17]. However, Godshall [18] discovered that there is no influence of sugars on the VLE of flavours in beverages containing minor concentrations (≤ 15%). Other authors [19-21] could also show that there is no significant influence on the VLE of flavours in water at carbohydrate concentrations up to 20 %. Lubbers et al. [22] showed that the influence of proteins in small amounts is also negligible. The authors asserted that flavour components in foods containing more than 50 % of water are present in such a high dilution that this corresponds with a good approximation to the state of infinite dilution in pure water. Because of this, the VLE of a flavour component in wort can be regarded as a VLE between the flavour component and pure water. This fact will be proven in the mentioned follow up article in this journal.

As alluded, the VLE in a state of infinite dilution can be described by limiting separation factors (K_i^{∞}). Limiting separation factors are measures of the vapour liquid equilibrium behaviour of strongly diluted solutions, such as aroma compounds in water (wort). The limiting separation factor of a component in water is only a function of the temperature [12]. Thus, this factor stays equal if the temperature does not change. As the latter is valid for the boiling of wort at constant ambient conditions, the limiting separation factors of wort flavour components stay equal during the whole procedure. In such high dilutions, the VLE-curve at a given temperature is linear and can be described by the following equation (Eq. 1):

$$y_i(x_i) = K_i^{\infty} \cdot x_i \qquad (1)$$

where $y_i(x_i)$ is the concentration of the component i in the vapour phase, and x_i the concentration of the same component in the liquid phase (e.g. wort).

3 Materials and methods

Description of the used still

The liquid x_i and vapour y_i compositions, as well as the values for pressure and temperature, were obtained from measurements made with a recirculating still of the Gillespie-type [23]. The used equilibrium apparatus was an all-glass, dynamic recirculating still (Labodest VLE 602 D, "Fischer Techology", Bonn, Germany), equipped with a Cottrel Pump [24]. A scheme of the used apparatus is given in figure 1.

The producer [25] gives an uncertainty in the measurement of the temperature of ± 0.1 °C. The apparatus is equipped with a glass temperature probe PT 100 having an uncertainty of ± 0.08 °C at 100 °C. The pressure in the still is measured with an uncertainty of ± 1 mbar according to the manufacturer. The still is able to work in a broad range of pressure and temperature and is described in detail elsewhere [26].

The following gives a brief description about the basics of the recirculating still: Vapour is continuously generated in a vessel (fig. 1:1). Due to the Cottrell Pump, liquid is entrained with the arising vapour into the equilibrium chamber. In this chamber, the vapour and the entrained liquid are separated. The vapour continues to rise and is condensed afterwards. The vapour condensate circulates back into the sample pot (fig. 1:2) via the condensate backflow way (fig. 1:8). The liquid separated in the equilibrium chamber circulates directly back into the sample pot via the liquid backflow path (fig. 1:9). Both backflows are mixed in the sample pot and evaporate again. As there are two recirculating phases that are in strong contact with each other, equilibrium is reached after certain times. During this procedure, the temperature and the pressure in the equilibrium chamber are measured. After equilibrium has been reached between the two phases, samples of the condensed vapour phase and the liquid phase are taken (fig. 1:6/7) and their compositions are analysed [24].

Procedure of the measurements

Volumetrically prepared solutions (10 µL/L to 40 µL/L) of the investigated wort flavour components in water were placed into the boiler and the electrical heater was turned on. Although less than 4 h are generally sufficient to establish a steady state [27] due to the expected strong deviation from ideal behaviour, boiling was continued for 7 to 8 h. The measurements were repeated five times with different solutions. Since the aqueous solutions were highly dilute, their boiling temperature was practically indistinguishable from that of pure water.

The producers and the purities of the chemicals used for the measurements are given in table 1 together with their CAS numbers.

Sample analysis and resulting limiting separation factor (K_i^{∞})

Since there is a strong absorption of UV light exhibited by the compounds phenylethanal, 2-phenylethanol, 2-furfural, γ-nonalactone and benzaldehyde, the compositions of the liquid and the condensed vapour phase were analysed using a Milton Roy spectrophotometer, "Spectronic 1201". The absorbance (Abs_{y_i / x_i}) was measured at pre-determined absorption maxima. While the equilibrium liquid phase samples were used directly for the measurements, most samples of the vapour phase condensate were measured after appropriate dilution so that the absorbance was situated in the ideal absorption range of 0.1 to 1.0 as recommended by Kortüm [28]. Silica glass cuvettes from "Hellma" (type 117.104-QS) with an optical length of 10 mm were used. The measurements were performed in the differential mode against pure water. In the limit of this high dilution, the ratio of the vapor y_i and the liquid equilibrium mole fractions provided the limiting separation factor (K_i^{∞}). Dohnal et al. [27] showed that since proportionality

relationships between the absorbance and concentrations of highly diluted solutions are known to exist, there is no need to calibrate the analytical response and thus the limiting separation factor (K_i^∞) is directly obtained as a ratio of absorbance of the equilibrium vapour- and liquid-phase samples (Eq. 2):

$$K_i^\infty = \lim_{x_i \to 0} \frac{y_i}{x_i} = \lim \frac{\mathrm{Abs}_{y_i}}{\mathrm{Abs}_{x_i}} \qquad (2)$$

For the other investigated components (DMS, 2-methylbutanal, 3-methylbutanal and hexanal), the absorption of UV light is too low for the analysis via the spectrophotometer. Thus, the determination of the concentration of the samples was performed using gas chromatographic analysis, which was carried out at the "Research Center for Brewing and Food Quality" [29]. This laboratory has a long lasting experience with the analysis of wort flavour components.

The carbonyl-components in wort were analysed according to method "PVGC 022", a proven and standard method for the analysis of wort aroma compounds. The method is described in detail elsewhere [30-32]. The following gives a brief description of this method together with the GC parameters: The volatile compounds of wort are enriched by steam distillation and extracted with dichloromethane. Afterwards, the solvent phase is analysed gas chromatographically using a flame ionisation detector (FID). The verification of the detector's linearity and the determination of the concentration occurs via several concentration levels within the relevant area, under evaluation of the relative peak areas. The GC parameters of this method and a demonstration of a chromatogram for carbonyl components in wort is given in the preceding article [1].

The compound DMS was analysed according to "MEBAK III". The method has been described previously in detail [33]. The following gives a brief description of the method "MEBAK III" together with the GC parameters: DMS in wort is also analysed gas chromatographically using head space technique together with a flame photometer detector (FPD). The determination of the concentration occurs via several concentration levels within the relevant area under evaluation of the relative peak heights. The GC parameters of this method and a demonstration of a chromatogram for DMS in wort, including an internal standard, is given in the preceding article [1].

The limiting separation factor of the components analysed by gas chromatography was directly obtained by the ratio of the analysed mole fractions of the liquid and vapour samples (Eq. 3):

$$K_i^\infty = \frac{y_i}{x_i} \qquad (3)$$

4 Results and conclusion

The results of the measurements are shown in Table 2 together with their confidence intervals (95 %), as well as the limiting separation factors of the same components that could be found in the literature to the best of the authors` knowledge. In the literature [34, 35], only the standard deviations of the measurement results were given. To be able to compare the literature values with the values of this work, the confidence intervals of the given literature values had to be calculated out of the standard deviations first. A detailed description of such a calculation is given elsewhere [36]. Because of this, the calculated confidence intervals (95 %) of the limiting separation factors taken from the literature are given in this article, which is in contrast to the literature [34, 35].

Table 2 shows that there are huge differences in the magnitude of the K_i^∞-values of the flavours investigated. As expected, all flavours that can be easily evaporated during the boiling of wort have also a large limiting separation factor (e.g. DMS, 2-methylbutanal, 3-methylbutanal, hexanal). In opposite to this, flavours that can hardly be evaporated during the boiling of wort have a smaller K_i^∞-value.

The result for 2-furfural is astonishing. Against the popular opinion that 2-furfural is only recreated and not significantly evaporated during the boiling of wort [37], its K_i^∞-value is much higher than those of some other investigated flavours. Because of this fact, 2-furfural can be easier evaporated during the boiling of wort than the compounds with a lower separation factor. The compound 2-furfural is a routing substance of the wort`s thermal load that can be expressed by the thiobarbiture acid value (TBZ) [38]. Because of this, it is possible to reduce the TBZ during the boiling of wort, if the evaporation rate is set up closer to the recreation rate.

Table 2 shows further that there is no significant influence of small differences in the ambient pressures on the limiting separation factors. Small differing boiling temperatures have no significant effects on the K_i^∞-values for all of the investigated compounds that could be also found in the literature. The K_i^∞-values of each compound of this work and of the literature are overlapping within their confidence intervals.

Unfortunately no data for hexanal, 2-methylbutanal, 3-methylbutanal and DMS could be found in the literature. Thus, the data of this article cannot be compared with limiting separation factors at 1013 mbar. As all other investigated compounds showed no differences in their values compared to literature data, it can be assumed that there is also no significant influence of small changes in the ambient conditions on the K_i^∞-values of hexanal, 2-methylbutanal, 3-methylbutanal and DMS. As a result, it can be stated that the location of a brew house has no significant influence on the VLE of flavours during the atmospheric boiling of wort. So there is no difference in the calcination of flavours between a brew house located in the mountains or at sea level.

5 Summary

The VLE of important off-flavour components in wort was determined in this article in form of limiting separation factors in water at the atmospheric boiling temperature of wort. If the results of this work are combined with the results of a preceding article [1], which focused on the recreation of the same compounds at the same temperature, it is now possible to calculate residue curves of flavours during the atmospheric boiling of wort. In the case of wort boiling, these residue curves give a relationship between the percentage decrease of a flavour and the percentage evaporation of wort. Because of this, it is now possible to calculate a needed over-all evaporation if the VLE, the required concentration of a compound at the end of boiling, and the initial concentration of the compound in the kettle up wort are known. This calculation can be made individually for each brew.

The results show further that there are large differences in the amount of the limiting separation factors of the investigated compounds. The lowest limiting separation factor has been observed for 2-phenylethanol (2,21 ± 0,06). The component with the highest limiting separation factor is dimethylsulfide (75,6 ± 6,4). The result for 2-furfural is astonishing. Against the popular opinion that 2-furfural is only recreated and not significantly evaporated

during the boiling of wort [37], its limiting separation factor is quite high (7,30 ± 0,14). Thus, it can be significantly evaporated during the boiling of wort. Because of this, it is possible to reduce the TBZ during the boiling of wort, if the evaporation rate is set up closer to the recreation rate.

A comparison of the results of this article (temperature range: 98,1 - 99,0 °C) with literature [34, 35] data at 100 °C shows, that the location of a brew house has no significant influence on the VLE of flavours during the atmospheric boiling of wort. So there is no difference in the calcination of flavours between a brew house located in the mountains or at sea level. The results of this and of the preceding article will be used in a follow up article in this journal, dealing with the residue curves of the same flavours at the atmospheric boiling of wort. The calculated residue curves will be proven with experimental decreasing values.

6 Literature

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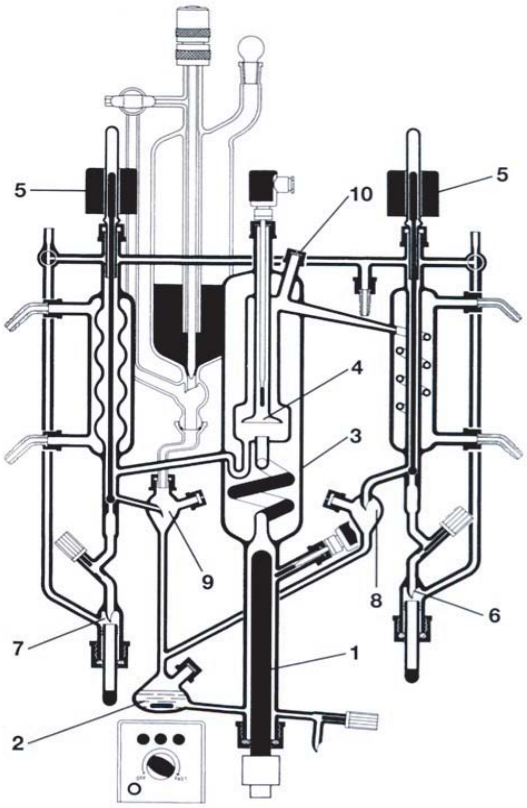
Received 12 October, 2006, accepted 4 December, 2006

Appendix



1 = Heater and vessel

2 = Sample pot

3 = Vacuum jacket

4 = Temperature measurement

5 = Magnetic valve

6/7 = Sampling of condensate/liquid

8 = Condensate backflow

9 = Liquid backflow

10 = Sampling of steam

Fig. 1 Scheme of the used recirculating still [9]

Table 1 Description of the used chemicals

Component	Producer	CAS-Nr.	Purity
Dimethylsulfide	Merck	75-18-3	≥ 99 %
Hexanal	Merck	66-25-1	≥ 98 %
2-Methylbutanal	Fluka	96-17-3	≥ 90 %
3-Methylbutanal	Merck	590-86-3	≥ 98 %
Benzaldehyde	Merck	100-52-7	≥ 99 %
2-Furfural	Merck	98-01-1	≥ 99 %
2-Phenylethanal	Acros	122-78-1	≥ 98 %
γ-Nonalactone	TCI Europe	104-61-0	≥ 98 %
2-Phenylethanol	Merck	60-12-8	≥ 99 %

Table 2 K_i^∞ -values acquired in this work compared to those from the literature

Component	K_i^∞	K_i^∞ (Literature)
Dimethylsulfide	75.60 ± 6.40	-
2-Methylbutanal	57.50 ± 6.10	-
3-Methylbutanal	55.50 ± 5.90	-
Hexanal	48.30 ± 6.20	-
Benzaldehyde	21.90 ± 0.40	20.80 ± 0.90 [34]
2-Furfural	07.30 ± 0.14	07.54 ± 0.24 [34]
Phenylethanal	05.57 ± 0.28	05.32 ± 0.17 [35]
γ-Nonalactone	03.11 ± 0.13	03.10 ± 0.08 [34]
2-Phenylethanol	02.21 ± 0.06	02.28 ± 0.07 [35]