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Approach to an inline monitoring of the heat impact in a high temperature short time treatment (HTST) of juice with the help of a chemical marker

The conventional method for the determination of the lethal heat load during pasteurisation (expressed in so-called pasteurisation units (PU)) by measuring temperature and flow rate provides known inaccuracies and requires safety margins in terms of a planned over-pasteurisation to the detriment of the product quality. Based on the hypothesis that chemical conversions correlate with applied heat input, despite the differences in reaction kinetics between chemical conversion and microbiological inactivation, inline near infrared spectroscopy (NIRS) was investigated to identify and quantify applied PU. Acid hydrolytic sucrose degradation was confirmed a favourable marker reaction. In a first step by still using offline analytics (HPLC) and a calculation the feasibility and plausibility in principle could be proved. Compared with conventional PU deviation of only 0.3 % were found when using the chemical marker reaction. However, the inline application using NIRS showed too high variations. The too low accuracy of the NIRS model for the sucrose measurement was identified of being the cause for failing the overall goal. Improvements in the inline determination seem to be promising.

Descriptors: near infrared spectroscopy, apple juice, pasteurisation, acid hydrolytic sucrose degradation, inline measurement of heat input, pasteurisation units

1 Introduction

Beverages, such as fruit juices, are often preserved by thermal treatment in continuous pasteurisation plants. The most important objective of this step is to guarantee microbiological safety, whereby large safety margins and known inaccuracies must be applied [1, 2]. The usage of empirical-based formulas for calculating the amount of required heat input (expressed in pasteurisation units (PU)) leads to rough generalisations because of inconsideration of heating and cooling sections as well as product-specific properties. The general formula for calculating the PU value is given in equation 1 with the time (t [min]) for which a certain temperature (T [°C]) was hold [1]. The theoretical basis of this simplified formula is the so-called D-value. It is a measure of the heat resistance of microorganisms and is given in minutes. This time indicates how long it takes at a defined temperature to reduce the initial microorganism count to one tenth. The D-value is specific for the various microorganism species and also for the environment in which they are found. For certain product groups, however, they can be generalised, as has been done with regard to fruit juices, for example. Here, specific constants are assumed and specified, which in turn contribute to a more unspecific pasteurisation, as the product properties are left out as mentioned above [3, 4].

$$\mathrm{PU} = \mathrm{t} \cdot 10^{\frac{\vartheta - \vartheta_B}{z}} \qquad \text{(Eq. 1)}$$

The z-value defines the temperature increase compared to the reference temperature ($\vartheta - \vartheta_B$) which provokes a decrease of the D-value by one order of magnitude. The kind of microorganism (strain) and the habitat conditions influence the z-value. However, for fruit juices a z-value of 10 K is typically used in practice by convention (so-called fruit juice formula) [3, 5, 6]. The applied temperature is ϑ, the reference temperature ϑ_B for fruit juices is by convention 80 °C [7].

The use of this formula with globalised values leads on the one hand to a high degree of safety in terms of microbiological stability, but on the other hand is also accompanied by adverse product changes regarding nutritive and sensory properties. With the knowledge of the negative effect of heat on the value-giving ingredients of fruit juices, there is no need to explain that such safety margins should be reduced as far as possible. Otherwise vitamins and antioxidants are degraded unnecessarily, colour changes and other physiochemical modifications occur [8–12]. Many studies deal with the observation of changes in fruit juices during thermal treatment, such as ascorbic acid degradation, colour and flavour changes or the formation of hydroxymethylfurfural [13].

https://doi.org/10.23763/BrSc21-20weishaupt

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The aforementioned facts give reasons for the goal of turning away from the current method of PU determination. A prior attempt aimed to make latent, nonspecific chemical changes, caused by heating, directly measurable using inline near infrared spectroscopy (NIRS). In combination with chemometric methods, an attempt was made to determine the thermal load expressed in PU [14]. However, using this method, the microbiological impact could only be determined with sufficient accuracy limited to a case specific application. For the use of, for example, a different beverage, the underlying model must be adapted. The limitation of this approach leads now to a modified approach undertaken in the present study. Here, also previous research on the sucrose hydrolysis as a chemical marker in pasteurisation was brought in [15]. The earlier studies on sucrose hydrolysis showed that the chemical marker reaction (sucrose degradation to fructose and glucose) can be used to measure heat input accurately in the course of thermal treatment [2, 15, 16]. The studies also showed that the traditional method of PU determination using temperature and time are comparably inaccurate.

However, the use of these markers is limited to studies outside of the real production operation (offline) and using artificial test solutions that are not comparable with real products (especially pH). In the present work now, the attempt is made to apply this chemical marker system in the process as inline method in a real product (apple juice). The challenges are hence that real products are used and thus the marker conversion cannot be artificially adjusted by the matrix properties (particular pH value) as in the former work. NIRS is used as the inline measurement method. Many studies work on with NIRS in combination with chemometric methods as analytical tool, but mostly in offline mode. Thus, the use of NIRS in combination with chemometrics has already proven to be a suitable method for such applications, such as fruit juice analysis both in-line and off-line [12–17].

As a part of the working hypothesis, NIRS is assumed to be capable for an inline sufficient quantification of sugar composition changes that take place and to assign them to a specific heat impact based on previously created models. In the next step, this must then be converted into the PU relevant for microorganism inactivation with the aid of kinetic data (z-values). With the knowledge of the changes in chemical composition, particularly the sucrose content, caused by a certain thermal stress, the heat impact, expressed in the “chemical” PU value, is supposed to be predictable. For the transformation from chemical reaction data to those of microbiological, also the reaction kinetics of the acid hydrolytic sucrose degradation are used. Finally, the hypothesis is that the lethal heat input in terms of the “microbiological” PU value, can be determined with the help of the chemical marker reaction of the sucrose degradation in an inline setup (called “chemical” PU). Consequently, the work of this study comprises two research questions. The first question is, if the extent of the chemical conversion of sucrose (acidic hydrolysis) in the real juice is sufficient (high enough) for an adequate indirect determination of the lethal heat impact (PU). Sufficient means here in comparison to the conventional PU derived from the process data temperature and flow rate (residence time). In this first part of the investigation, the sucrose is still analysed off-line in the laboratory by HPLC. The second research question derivated from the working hypothesis wants to know how the accuracy of the finally determined PU is impaired when the sucrose determination is transferred into an inline measurement with the help of NIRS and a chemometric model.

2 Material and Methods

2.1 General approach

Apple juice was pasteurised in a in a pilot scale flash pasteuriser. In this high temperature short time process (HTST) selected different settings for flow rate and temperature enabled the variation of the heat impact. Process data as temperatures, flow rates, system volume were measured and samples were taken beforehand the heat treatment and afterward in order to analyse the sucrose concentration changes. The correlation of sucrose concentration and heat impact provided a regression model that allowed to determine the here newly introduced “chemical” Pasteurisation Units (PU_{chem}) from the sucrose content. The PU_{chem} are dedicated to serve as an auxiliary calculation figure. For the calculation of the PU_{chem}, equation 1 is taken as for the “microbiological” PU. However, for

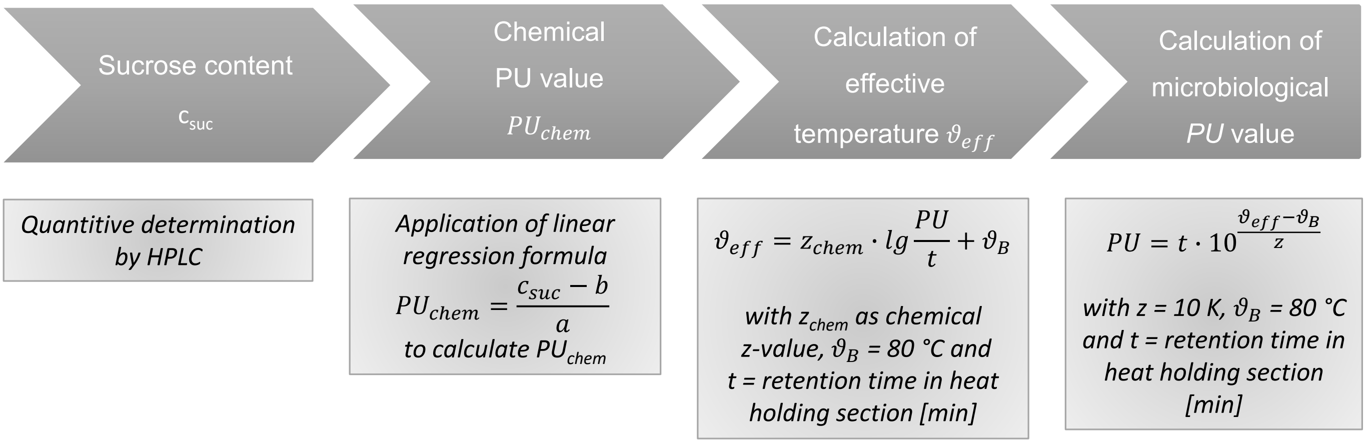

Fig. 1 **Approach to the first research question: Indirect calculation of “microbiological” PU values by using the (offline) sucrose concentration measurement with a HPLC; with c_{suc} as sucrose content in g/L and with a and b as slope parameter and axis intercept of a regression function**

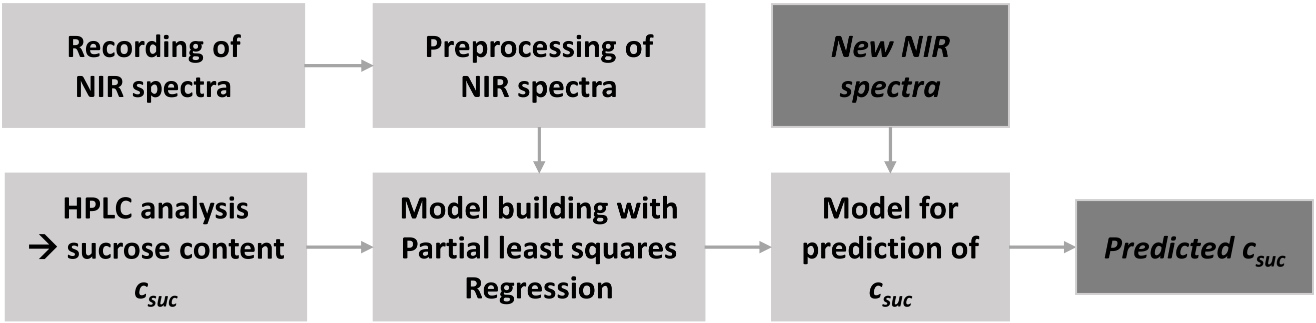

Fig. 2 Scheme of the procedure from the measurement of NIR spectra to Partial Least Squares Regression modelling and prediction of sucrose content

the purpose of this paper, the PU_{chem} employ the activation energy E_A of the sucrose hydrolysis and acidic environment instead of the "microbiological" z-value of 10 K (as used in fruit juice formula). In order to obtain a PU_{chem} the sucrose hydrolysis specific "chemical" z-values were determined with the help of the subsequent formula derived in several steps from the Arrhenius equation [15]. A separate "chemical" z-value had to be calculated for each pasteurisation temperature adjusted in the process settings, as the z-value depends on the temperature (applying equation 2).

$$z_{chem} = \frac{\ln 10 \cdot R \cdot \vartheta_{ref} \cdot \vartheta}{E_A} \quad \text{(Eq. 2)}$$

Here, R is the ideal gas constant ($8.314\,\frac{J}{mol \cdot K}$) and ϑ is the absolute temperature [K]. The activation energy E_A for the sucrose hydrolysis used is $105.09\,\frac{kJ}{mol}$. In a previous work mean E_A of $105.09 \pm 1.07\,\frac{kJ}{mol}$ (95 % confidence interval) were found [17]. Thus, the z-value is also temperature dependent, which leads to slightly different "chemical" z-values for the PU_{chem}.

The regression model of the sucrose concentration as a function of PU_{chem} was then used to approach the first research question. The measured sucrose concentrations from pasteurisation trials were taken to determine the PU_{chem} values for each run. Herewith, a so-called effective temperature (ϑ_{eff}) could be calculated. This is possible when the mean residence time is considered satisfactorily precise as it is derived from the flow rate measurement and the system volume. The adequacy of this premise refers to previous research for low viscous fluids [16]. Finally, the "microbiological" PU were calculated by taking the conventional "microbiological" z-value of the fruit juice formula of 10 K. Figure 1 shows the calculation procedure. The result of the first step is the comparison of the PU traditionally determined by process data with the PU received indirectly with the help of the chemical marker.

In the second step, the NIR spectra acquired during the pasteurisation trials were used to obtain the sucrose concentration of unpasteurised and pasteurised apple juices (before and after heat treatment). All other steps of the first approach stay equal. However, beforehand a sufficient chemometric model for the determination of the sugar concentration from spectra had to be developed. In figure 2, the scheme of the workflow, from recording of NIR-data to the prediction of sucrose concentration, is shown. For evaluating the second research question, this procedure is the continued by the processing steps shown in figure 1.

2.2 Apple Juice Preparation and Heat Treatment

Apple juice was prepared freshly and was frozen at –18 °C directly afterwards in laboratory scale with apples procured at a local retail store (dessert apples). For the pasteurisation runs, apple juice was unfrozen. Heat treatment was realised in a laboratory HTST/UHT system type HT220 (OMVE Netherlands B.V., De Meern, Netherland). The heat impact (PU) was varied by changing the temperature (90, 100, 110 and 120 °C) in the heat holding section, the flow rate and the time of sampling. High levels of PU were also received by defined recirculating of the juice. Each parameter setting was run in a three-fold measurement. After heat treatment, the samples were cooled down to 20 °C for the analytical measurements.

2.3 Analysis of sucrose content as reference value

The content of sucrose of sample material was analysed in a three-fold measurement, from which an average value was calculated, resulting in a total of 48 mean concentrations. This was done automated by a high performance liquid chromatograph (HPLC) type Flexar FX-10 (PerkinElmer Inc., Rodgau, Germany) with a flow rate of 0.6 mL/min, using 5 mmol sulfuric acid in water as eluent. A Nucleogel Sugar 810 H separation column was used.

Table 1 Set process temperature and associated "chemical" z-values calculated with sucrose degradation kinetics

Process temperature [°C]	"chemical" z-value [°C]
90	23.386
100	24.030
110	24.674
120	25.318

Table 2 Overview of the various residence times [min] of the samples in the hot holding section

0.178	0.359	0.718	1.078	1.437	1.616	1.976	3.233	6.465	9.698	12.930	16.163

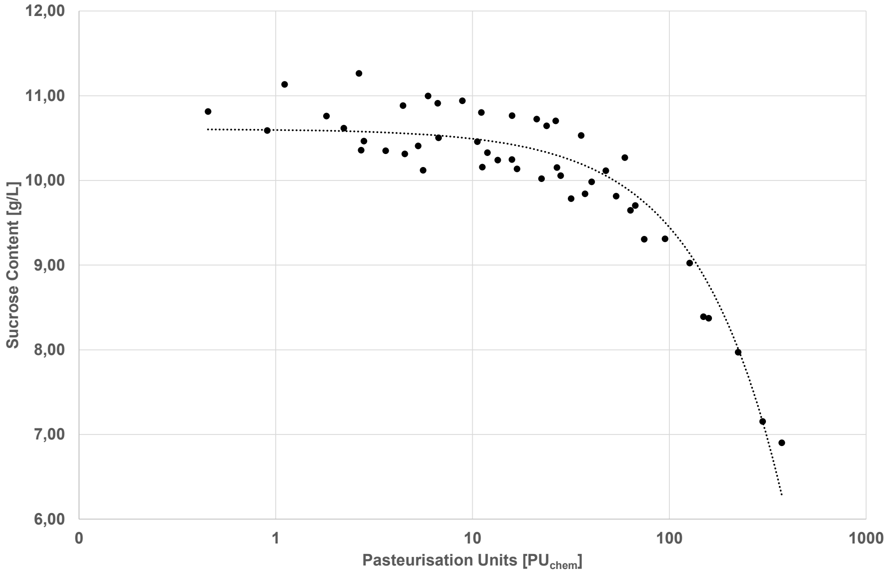

Fig. 3 **Regression curve of the sucrose content over the pasteurisation units PU_{chem} calculated with reaction kinetics of sucrose degradation with a reference temperature ϑ_B of 80 °C; $R^2 = 0.89$; the points correspond to the sucrose contents measured by HPLC at corresponding PU_{chem} values determined from process data; the line corresponds to the resulting regression curve with the equation** $c_{sach}\left[\frac{g}{L}\right] = -0.0116 \cdot PU_{chem}[min] + 10.608$

Table 3 **Selection of experimental results according to trials corresponding to figure 1 - indirect PU_{microb} derived from HPLC sucrose measurement (off-line) and with the help of a correlation between sucrose content and PU_{chem} (with E_A = 105.09 kJ/mol)**

calculated PU_{chem}	effective heating temperature	PU_{microb} indirect by Marker	PU_{microb} Friut Juice formula	Percentage deviation
[PU]	[°C]	[PU]	[PU]	[%]
2.8	85.6	5.9	5.9	0.0
5.6	85.6	11.7	11.7	0.0
11.2	85.6	23.4	23.4	0.0
16.8	85.6	35.1	35.2	0.3
22.4	85.6	46.8	46.9	0.2
28.0	85.6	58.5	58.6	0.2
6.7	94.9	49.4	49.5	0.2
13.4	94.9	98.8	99.0	0.2
26.8	94.9	197.7	198.1	0.2
40.3	94.9	296.5	297.1	0.2
53.7	94.9	395.4	396.1	0.2
67.1	94.9	494.2	495.2	0.2
15.8	104.5	451.8	452.0	0.0
31.7	104.5	903.6	904.0	0.0
63.4	104.5	1 807.3	1 808.0	0.0
95.1	104.5	2 710.9	2 712.0	0.0
126.8	104.5	3 614.5	3 616.0	0.0
158.5	104.5	4 518.2	4 520.0	0.0
37.2	114.5	4 552.7	4 555.4	0.1
74.5	114.5	9 105.3	9 110.9	0.1
149.0	114.5	18 210.7	18 221.7	0.1
223.5	114.5	27 316.0	27 332.6	0.1
298.0	114.5	36 421.3	36 443.4	0.1
372.5	114.5	45 526.7	45 554.3	0.1

2.4 Linear regression with the sugar content as a function of the "chemical" PU value

For each sample, a case specific PU_{chem} was calculated using the process data of temperature and retention time as well as case specific "chemical" z-value. A linear regression of these PU_{chem} values and the HPLC reference results for the sucrose content was performed.

2.5 NIRS and chemometric modelling

During flash pasteurisation of freshly pressed apple juice measurement of NIR spectra were made. The spectra were recorded by a spectrometer type PSS-2120 (Polytec GmbH, Waldbronn, Germany) in conjunction with a transflection probe type FDP-7UVIR200-2-VAR-BX (Avantes B.V., Apeldoorn, Netherland) with a path length set to 2 mm. Five measurement repetitions were carried out per sample. The recorded NIR spectra were preprocessed and analysed using the software Pas Labs 1.2 (Polytec GmbH, Waldbronn, Germany) by doing a Principal Component Analysis (PCA) to investigate systematic changes in the samples due to thermal treatment. In the PCA, a dataset of large size is mathematically reduced and transformed to generate a new system with a reduced number of linear combinations. This leads to the so-called principal component, which contains a maximum of the variance of the initial dataset. In addition, combining the NIR spectra with the results of the reference analytics (Y variable), a Partial Least Squares Regression (PLSR) was performed to evaluate the suitability of NIR as inline analytical tool for the sucrose content in apple juice. Using the PLSR, in addition to the X variable (individual wavelengths as measurement points), the Y variable (reference measurement values) is also projected into a new space and a search is made for correlations between these two spaces, i.e. the covariance. Similar to PCA, this method is preceded by a data reduction, but with the focus on maximum correlation. Both PCA and PLSR models are gradually optimised in an iterative process via the analysis of various quality parameters. For this purpose, preprocessing techniques such as wavelength selection, standard normal variation (SNV) as a standardisation method and the formation of the second derivative are applied. The coefficient of determination (R^2), the root mean square error of estimation (RMSEE) and root mean square error of cross validation (RMSECV) are used as quality parameters. Furthermore, the root mean square error of prediction (RMSEP) is determined with an internal test set. All these quality parameters are available in the unit of the Y-variable. With the PLSR model the sucrose content of unknown samples can be predicted.

3 Results

3.1 Correlation of sucrose degradation and "chemical" PU

A requirement for both research questions and their examination is the regression model for correlation of the sucrose content and the PU_{chem}. For this purpose, the PU_{chem} values were calculated previously from the process data (temperature and retention time) using the "chemical" z-values of the sucrose degradation with equation 1. Because the z-values themselves depend on the temperature, they were calculated for each process temperature by using equation 2 assuming the activation energy E_A of 105.000 $\frac{kJ}{mol}$ and the reference temperature T_B of 80 °C. The z-values and retention times in the heat holding section on which the calculation is based are listed in table 1 and 2.

Fig. 4 Exemplary NIR spectrum at 90 °C and 10 L/h after wavelength selection and SNV

Table 4 PLSR model properties and quality parameters for the sucrose content in g/L; with R^2 as coefficient of determination, Q^2 as predictive quality parameter and RMSEE, RMSECV and RMSEP as root mean square errors of estimation, cross validation and prediction in g/L

Parameter	$R^2(X)$	$R^2(Y)$	Q^2	RMSEE [g/L]	RMSECV [g/L]	RMSEP [g/L]
Sucrose	0.999	0.776	0.718	0.46	0.53	0.47

The combination of the four process temperatures and 12 heating times resulted in 48 test runs. Each run was performed as a threefold measurement and the resulting data were averaged.

The results of PU_{chem}, calculated with values in table 1 and 2 were then subject to a linear regression analysis together with the results of the sucrose content from the HPLC analytics. A linear correlation was obtained represented by a numerical value equation (regression coefficient of 0.89):

$$c_{sucrose}\ \left[\frac{g}{L}\right] = -0.0116 \cdot PU_{chem}\ [min] + 10.608 \quad \text{(Eq. 3)}$$

Figure 3 shows the regression graphically in a semi-logarithmic plot.

3.2 Proof of the chemical marker reaction for PU determination by off-line sucrose analysis

When the regression formula was determined, the "microbiological" PU values (PU_{microb}) were calculated according to the scheme in figure 1. In table 3 there is a selection of the results of the 48 pasteurisation experiments. The PU_{chem} values were obtained by inserting the sucrose contents into the regression formula. From this, the effective temperature was calculated according to figure 1. This in turn was then converted into the PU_{microb} values (third column). In this calculation sequence, slight deviations from the set process temperature can already be seen in the effective temperature. Consequently, the resulting indirect PU_{microb} differ from those PU_{microb} that are conventionally calculated directly with measured process data (temperature and flow rate) applying the fruit juice formula. However, for the PU values up to 100 PU the relative deviation ranges only between 0.0 % and 0.3 %. So far, the first part of the hypothesis can be affirmed. However, the so far tried methodology is still not capable for real-time monitoring.

3.3 NIRS model for the sucrose concentration in apple juice used in the experiments

In the presented approach, NIRS was investigated for the identification of the chemical marker in terms of the sucrose concentration. Therefore, a PLSR model had to be built in advance. For each sample, five spectra were recorded, resulting in a total number of 720 spectra. Four of these replicates were processed within the model building and the fifth spectra of each sample was used for internal validation to calculate the RMSEP. From the entire wavelength range, the ranges of 1108 – 1397 nm and 1501 – 1858 nm were used and the Standard Normal Variation (SNV) preprocessing method was applied. Figure 4 shows a typical spectrum after preprocessing.

An iterative process of model building resulted in a PLSR model with 13 latent variables (LV) including 576 spectra, model properties and quality parameters were shown in table 4.

The number of required LVs was verified for significance by a permutation test. Using the test set, the RMSEP value was calculated that represents the prediction quality. The results of the application

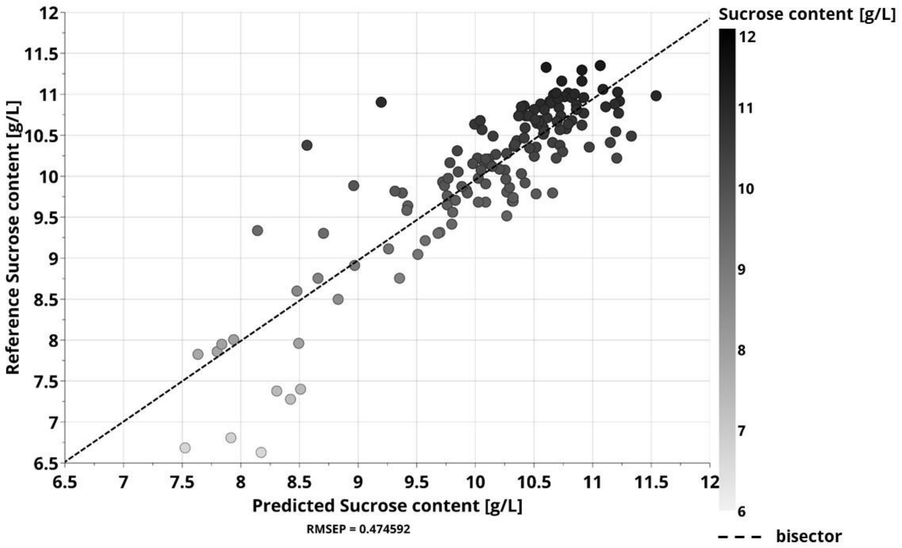

Fig. 5 Predicted versus reference sucrose content in g/L resulting from the PLSR model applied on the internal test set

Table 5 Results of "chemical" PU values reached by applying regression formula and predicted sucrose content; results of effective heating time and of "microbiological" PU values; in last column the percentage deviation of theoretical and practical PU calculation

predicted sucrose content	heating time	predicted PU_{chem}	effective heating temper-taure	PU_{Microb} indirect by marker	PU_{Microb} Friut Juice formula	Percent-age devia-tion
[g/L]	[min]	[PU]	[°C]	[PU]	[PU]	[%]
10.69	1.62	52.34	115.3	5 504	5.9	93 288
10.52	3.23	67.56	110.9	3 952	11.7	33 778
9.84	6.47	125.67	110.1	6 671	23.4	28 509
10.47	9.70	71.89	100.3	1 050	35.2	2 983
10.34	12.93	82.75	98.9	993	46.9	2 117
10.09	16.16	104.37	98.9	1 267	58.6	2 162
10.35	1.62	81.57	120.9	19 993	49.5	40 390
10.01	3.23	110.79	116.9	15 779	99.0	15 938
10.20	6.47	94.53	108.0	4 075	198.1	2 057
10.08	9.70	104.80	104.8	2 956	297.1	995
9.93	12.93	118.27	103.1	2 640	396.1	666
10.09	16.16	104.66	99.5	1 439	495.2	291
10.14	1.62	99.65	124.2	42 175	452.0	9 331
10.27	3.23	89.22	115.6	11 610	904.0	1 284
9.83	6.47	126.50	111.9	9 937	1 808.0	550
9.80	9.70	129.17	107.7	5 771	2 712.0	213
9.26	12.93	176.06	108.0	8 124	3 616.0	225
9.35	16.16	168.07	105.1	5 222	4 520.0	116
8.96	1.62	201.75	133.1	328 041	4 555.4	7 201
8.71	3.23	223.68	126.6	147 325	9 110.9	1 617
8.48	6.47	243.30	119.9	63 037	18 221.7	346
7.84	9.70	298.28	117.7	56 739	27 332.6	208
8.42	12.93	247.88	112.5	22 856	36 443.4	63
8.17	16.16	269.83	111.0	20 129	45 554.3	44

of the PLSR model on the internal test set are visualised in figure 5 as "predicted-versus-reference" plot.

3.4 Proof of the chemical marker reaction for PU determination by NIRS inline measurement

After the basical feasibility was proven by offline analytics, the approach was performed inline with practical data. Instead of HPLC analysis, NIRS is now used to determine sucrose concentration. After running through the individual calculation steps shown in figure 1 and 2, significant and relevant deviations of PU_{microb} values indirectly determined by NIRS from the conventionally measured PU_{microb} were found. Overall, the indirectly calculated values are higher than those calculated directly with the use of process data. Results are shown in table 5.

The large deviations result most likely from the prediction errors of the NIR measurement. This had an insufficient accuracy and as a result, errors in the inline sucrose prediction have a strong propagation effect on the overall result. Therefore, the theoretically feasible approach of indirect PU determination using NIRS as an inline analysis tool could not be implemented in practice. A more precise measurement of the sucrose content, even in the low change range, would be required to realise this type of PU value determination. With such an analytics tool, however, the approach would be feasible, which could be shown within this study.

4 Discussion

As to the first part of the working hypothesis, it can be affirmed that the sucrose hydrolysis can serve as chemical marker in apple juice capable for the quantification of the microbiologically effective heat impact expressed in pasteurisation units PU_{microb}. This can be stated when comparing the PU with those derived from the conventional fruit juice formula. In the range up to 100 PU, which is the relevant range for practical juice pasteurisation's, the relative deviations of both PU_{microb} values (indirect from the chemical marker and by fruit juice formula) can be considered being negligible from a practical point of view. For example, Byssochlamys nivea ascospores with a decimal reduction rate (D-value) of 15.7 min (80 °C) [18] receives logarithmic count reduction of 3.18 applying

50 PU in purely mathematical terms. Assuming pessimistically the maximum all the found deviation 0.3 % resulting in a possible span of 48.6 PU to 51.4 PU the logarithmic count reduction ranges between 3.10 and 3.27.

In the second part of the work, the idea was transformed into an inline method. In contrast to the first part, drastic deviations between the indirectly measurement PU (NIRS and chemical marker) and the conventionally measured PU (flow rate and temperature) were found. The premise of this work is that both PU_{microb}, conventionally measured and indirectly determined with the help of NIRS in the marker reaction do differ to each other. Moreover, the assumption is that an indirect measurement can more precisely correspond to the actual heat impact on the microorganism. Even so, the deviation found deviates in an extent that the indirectly determined PU reveal being less credible. Even if the inline detection of the PU failed, a continuation of the approach seem to be promissing. In case the chemometrical model could be improved and the inline detection is implemented in a holistic renewal of the pasteurisation process which incorporates the case individual use of kinetic inactivation data (particularly strain individual z-values) the pasteurisation process would be much more precise than before. Those kinetic data are hardly already available on at least one internet accessible databases [7]. The globalisation of the z-value might be the most sensitive factor in the determination of the microbiologically effective heat impact. As for instance, a heat treatment of the afore mentioned Byssochlamys nivea ascospores applying 95 °C for 1.6 min adds up to 50 PU by taking the fruit juice formula with the z-value of 10 K. Experimentally, the found z-value for this strain was 4.5 [18]. When applying this real z-value the resulting heat load is 3500 PU. In view of these considerations, the found deviations in the inline detection by NIRS are not eliminated but diminished. The findings of the present study, in which the newly demonstrated approach was examined, initially refer to the product category of fruit juices, which consist to a certain extent of sugars. Although the results cannot be directly transferred to the product category of plain beers, they can in related areas. In the category of mixed beer beverages and certain non-alcoholic beers, however, the conditions, namely the presence of sugars, are given, so that the findings are considered to be so far relevant for the beer industry. If the superordinate finding that a chemical reaction is used as a marker reaction is considered, there is also potential for research for an application in plain beers. If a chemical marker reaction can be identified that takes place in the beer in the course of thermal treatment, this approach could be transferred and would offer optimisation potential for the thermal preservation.

5 Conclusion

A new method to determine the effect of thermal treatment expressed in pasteurisation units (PU) was approached in two steps (offline and inline). The chemical marker reaction sucrose hydrolysis achieved in the offline procedure deviation of 0.3 % for the pasteurisation of apple juice. So far, the chemical marker reaction seems to be plausible and comparable in the practically relevant PU range up to 100 PU. However, practical relevance gains the novel method only if it can be transferred into an inline measurement. The therefore investigated second step using near infrared spectroscopy (NIRS) did not yet sufficiently succeed. This is due to the quality of the NIRS measurement and the resulting model quality of the chemometric models used. Since the principle of the approach could be proven to work (offline), improving the accuracy of the inline sugar measurement would lead to an overall successful new method. In spite of some difficulties, mid-infrared spectroscopy for the inline application could be worth to investigate in this instance. In a larger context, the application of inline sensors in the pasteurisation process has a great potential for a more individualised treatment, particularly when the global z-value in the applied fruit juice formula can be substituted by product specific z-values. Considering results obtained with the conventional z-value, the large deviation found in this work for the inline application can be put into perspective.

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Received 26 November 2021, accepted 21 January 2022