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Aquaphotomics assessment for the physicochemical properties of lemon juice

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Abstract

The field of aquaphotomics, which focuses on water's interactions with biomolecules, has emerged as a powerful tool for assessing citrus juice quality. By using advanced spectroscopic methods like near-infrared (NIR) and Raman spectroscopy, researchers uncover water-solute associations. This non-destructive technique provides valuable insights into lemon juice properties, including pH, TDS, EC, Brix, and RI. Additionally, aquagrams—a visual representation of absorbance levels—reveal water composition across different wavelengths. The present work focuses on assessment of physical and chemical properties of lemon juice using the aquaphotomics range. 29 lemon juice samples were extracted and their physicochemical parameters and spectral data were assessed. The water matrix coordinates lying in the aquaphtomics range were analysed and it was observed that wavelengths from 1438 to 1513 nm were very important for the analysis for the analysis of quality of citrus juices.

Keywords: lemon juice, aquaphototmics, physicochemical parameters.

Introduction

Near Infrared (NIR) spectroscopy had been used as a non invasive, green and rapid technique for the quantitative and qualitative analysis, authentication of the food products and beverages. NIR spectroscopy involves the interaction of electromagnetic radiation with water molecules in the near-infrared region of the spectrum (typically 780-2500 nm). This technique may be limited to understand the qualitative changes in water molecular matrix, but the upcoming concept of aquaphotomics have become a non-destructive method for the spectral

measurements of the water matrix coordinates. Aquaphotmics in collaboration with the multivariate analysis have been useful in assessing the perturbation in the water coordination in water contained food and beverages [1].

Aquaphotomics is an emerging field that focuses on the study of changes of water bonds in the near-infrared (NIR) spectra. Aquaphotomics understands the complex interactions between water molecules and other components present in a sample, providing valuable information about the composition, properties and authentication of the sample under study [2]. This phenomenon can be used for the analysis of water quality, including the detection and quantification of impurities, contaminants, and dissolved substances. This is particularly useful in qualitative and quantitative analysis of products. It was also reported by different researchers across the world that the aquaphotomics approach is useful in investigation of quality of water. It was observed that aquaphotomics approach in NIR spectra was successful in differentiating between different type of bottled water. The variation could be observed due to different concentration of minerals in water from various sources which could be identified in aquaphotomics approach [3].

Aquaphotomics have a potential of non-destructive which can be used for analysing the citrus juices without altering or damaging the samples [4]. The technique can be used for quality assessment of the citrus juices, identification of changes in water molecular patterns may indicate variations in sugar content, acidity, electrical conductivity, total dissolved solids and other quality parameters [5]. Aquaphotomics can be used to verify the authenticity of citrus juices by analysing their water molecular profiles. It can also be used to develop distinct aquaphotomics signatures for different varieties of citrus fruits and different processing methods [6]. Application of aquaphotomics were observed in research reported in 2022 where spectra was used to classify and quantify the stingless bee honey. Reported results showed that the aquaphotomics range, related to water properties and colour could be used to effectively discriminate the adulterated sting bee honey from the pure honey samples [7].

Citrus fruits are an excellent source of essential nutrients, vitamin C and minerals like potassium, magnesium, phosphorous, iron and calcium. From the ‘Rutaceae’ family, citrus fruits are widely grown fruit in the world with approximately 4 million tons production in 2022 in India [8]. Citrus juice offers numerous health benefits - protect cells from damage, supports the immune system, and aids in the absorption of iron, prevent common illnesses like colds and flu, antioxidant activity contributes to overall health and may reduce the risk of chronic diseases, lower blood pressure and improved cardiovascular function and contributes to overall nutritional balance [9].

Quality parameters of citrus juices – namely lemon have been assessed by various analytical, spectroscopy and chromatographic analysis. Physicochemical properties namely taste evaluation, ratio of sugar and acid, total soluble solids, total acidity of different orange juices from Korea, were analysed. The properties were assessed using the sensory evaluation methods [10]. Analysis of a healthy fruit drink was performed by the researchers in 2021 to formulate a beneficial health drink for the consumers. Analysis of physical, chemical, nutritional and sensory properties of mixed citrus fruit juice were analysed. The results showed that the mixed juice formulated with mixture of orange, lemon, ginger and honey was nutritious and beneficial for the health of consumers [11]. Another research was also reported in literature where a

handheld infra-red spectrophotometer was used to detect the adulteration in lime juices. Range of 900-1700nm with k-nearest neighbors was used to assess the authentication of citrus juices. Reported results showed that the model was successful in authentication of citrus juices and required a greater number of samples for the study to increase the robustness of the model [12]. The results reported in the literature showed that infrared range is useful in assessing the quality of citrus juices. But no or minimal research was found which used aquaphotomics for the assessment of citrus juice samples.

In the present research physicochemical properties and infrared spectra of the Lemon juice were measured and studied. The results were analysed to assess the physical and chemical properties of lemon juices using the Aquaphotmics range of infrared spectra. An effort was made to investigate the application of aquaphotomics for the assessment of lemon juice samples.

Material and methods

Sample Collection

Fresh lemon was procured from market and juice was extracted using handheld juice extractor. The extracted juice was sieved to get juice of specific particle size. Total lemon juice sample prepared were 29 in number. The prepared juice samples were used to measure the various physicochemical properties and near infrared spectra, within 30 minutes after the preparation of lemon juice samples. The samples were kept in glass beaker for the time before analysis and was not stored for long time to prevent the changes in the properties due to environment or temperature. The measurements were taken in triplicate and average of the same was taken for further analysis.

Physicochemical parameter measurement

The physical and chemical parameters namely – pH, electrical conductivity (EC), total dissolved solids (TDS) were measured using the digital meters in the laboratory at Lovely Professional University and ^{o}brix and refractive index (RI) were measured using the Abbe refractometer at the laboratory at Lovely Professional University.

Near infrared spectra

Near Infrared (NIR) spectra of the extracted juice samples were measured using the NIR DS 2500 spectrometer at CSIR – Central Scientific Instruments Organisation in transflectance mode using liquid sample holder with gold refractor. Spectra was collected in the range from 400 – 2500 nm with a gap of 0.5 nm in triplicate.

Statistical Analysis

The collected data of citrus juices for the physicochemical parameters and near infrared spectra was analysed using the descriptive statistics. Descriptive statistics helped in finding mean, median, standard deviation and variance for the physicochemical data of the lemon juice samples using Data Analysis- Addin in Microsoft Excel feature. The descriptive analysis helps in understanding the variation of the parameters for the lemon juice samples. Further aquagrams were developed using the water matrix coordinates and the properties were assessed using the selected wavelength ranges. Correlation analysis of the spectra in aquaphotomics range from 700-1000nm, 1000-1300nm, 1300-1600nm, 1600-1900nm, 1900-2200nm, 2200-2500nm with the physicochemical properties were studied.

Results and Discussion

Descriptive Statistics

The physical and chemical parameters of the 29 lemon juice samples are shown in Table 1. The physicochemical properties measured for 29-lemon samples - pH, TDS (in ppm), EC (in Siemens/m), ºBrix and RI were analysed by measuring their descriptive statistics are shown in Table 2. Results for the descriptive statistics namely – Maximum, minimum, mean, median, standard deviation, variance and standard error were calculated for lemon juice samples.

Table 1 Physicochemical parameters of lemon juice samples

Lemon	pH	TDS ppm	EC S/m	Brix º	RI
L1	1.7	2323	4.6	6	1.342
L2	1.7	2324	4.6	4.2	1.339
L3	1.7	2239	4.2	5.5	1.346
L4	1.7	2434	4.8	5	1.34
L5	1.7	2273	4.5	4	1.339
L6	1.8	2230	4.4	5.2	1.341
L7	1.9	2226	4.4	5	1.34
L8	1.7	2392	4.7	5.3	1.341
L9	1.9	2182	4.3	5.1	1.341
L10	1.8	2272	4.5	5	1.34
L11	2.2	2145	4.2	3.5	1.337
L12	1.8	2225	4.4	3.8	1.338
L13	1.7	2247	4.5	5	1.34
L14	1.7	2349	4.6	4.8	1.34
L15	1.8	2355	4.6	5.8	1.346
L16	1.9	2133	4.2	3	1.337
L17	1.9	2004	3.9	3	1.337
L18	1.8	2254	4.5	4	1.339
L19	1.8	2295	4.5	5	1.341
L20	1.6	2116	4.5	5	1.34
L21	1.9	2184	4.2	3	1.333
L22	1.8	2113	4.2	5	1.34
L23	1.8	2046	4	4	1.339
L24	1.8	2192	4.3	5	1.339
L25	1.8	1939	3.9	4	1.339
L26	1.7	2334	4.3	6	1.342
L27	1.7	2331	4.6	5.1	1.341
L28	1.7	2333	4.6	4.9	1.339
L29	1.7	2189	4.3	4.9	1.34

Table 2 Descriptive Statistics values for all the physicochemical parameters for lemon juice samples.

Statistics	pH	TDS ppm	EC S/m	Brix º	RI
Mean	1.783	2230.310	4.390	4.659	1.340
Standard Error	0.021	21.520	0.042	0.157	0.000
Median	1.800	2239.000	4.400	5.000	1.340
Standard Deviation	0.114	115.890	0.227	0.846	0.002
Sample Variance	0.013	13430.580	0.052	0.716	0.000
Minimum	1.600	1939.000	3.900	3.000	1.333
Maximum	2.200	2434.000	4.800	6.000	1.346

It can be observed from the standard deviation of pH, EC, Brix and RI for all the samples that there is less variation among each property value for same set of samples. Whereas for the TDS values, variation among the data set is high, which implies that there is large variation mong TDS from 1453 to 2434. Variation for the lemon samples for their pH, EC, TDS, Brix and RI were 1.78 ± 0.11, 4.39 ± 0.85, 2230.31 ± 115.89, 4.66 ± 0.85 and 1.34 ± 0.002 respectively.

Near Infrared Spectra

The raw and pre-processed spectra for the juice samples were observed and it can be observed that in the range of 900-1400 nm absorbance bands are observed where the spectra are flat after 2000nm, showing that the range of 2000nm contains complex spectra and is not significant for the determination of the quality parameters of the juice samples. Application of normalization and baseline correction helps in removing the noise from the sample spectra and clearly highlighting the important absorbance bands (Fig 1). Three ranges can be visualized from the spectra on the bottom left showing the wavelengths to be used for quality estimation. It can also be observed that the water matrix wavelengths are also highlighted in the spectra. Thus, the NIR spectra of the lemon juice samples clearly shows that the citrus fruits can be assessed using the absorbance spectral data and applying the pre-processing on it.

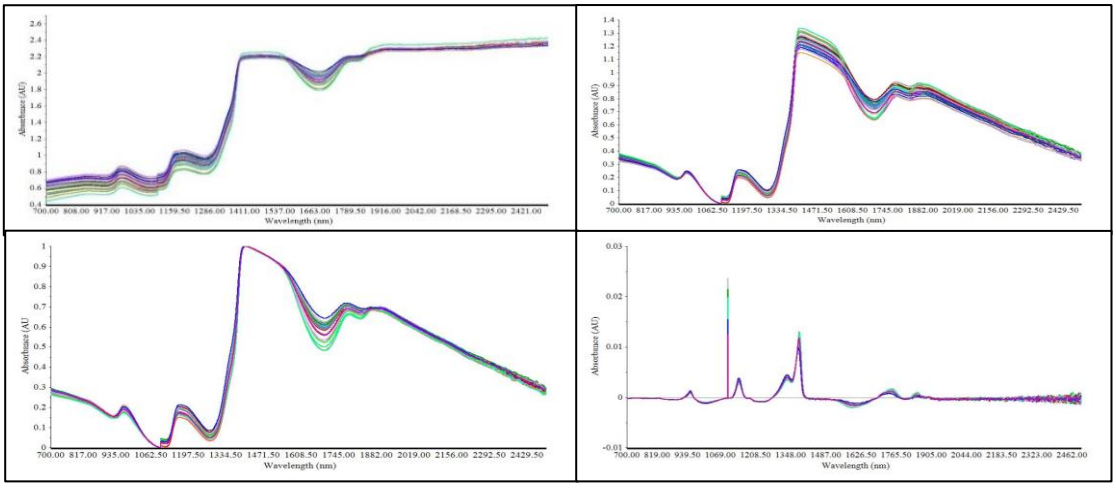

Figure 1 Near Infrared Spectra for the lemon juice sample – tope left : raw NIR spectra, top right : baseline correction, bottom left : baseline and maximum normalize and bottom right : 1st derivative preprocessing to the preprocessed spectra

Aquaphotomics Analysis

Aquagram is radar graph where the wavelengths are represented in the circle outline and their absorbance are shown by the concentric circles. Every line in the aquagram presents the absorbance of one sample for the complete aquaphotomics range. The absorbances of all the water matrix coordinates are represent in the form of aquagrams. To develop the aquagram one wavelength from each water matrix coordinates range is used, the 12 characteristics wavelengths in the first overtone region of water in NIR spectra used are – 1344nm (v3 streching of water bond), 1364 nm (water shell), 1372 nm (1st and 3rd vibration), 1382nm (water shell), 1398 nm (free OH), 1410 nm (S0), 1438 nm (HSO_2), 1444 nm (S1), 1462 nm (S2), 1474 nm (S3), 1492 nm (S4) and 1518 nm (v1 and v2) [13]. Aquagram for the lemon juice samples is presented in Fig 2.

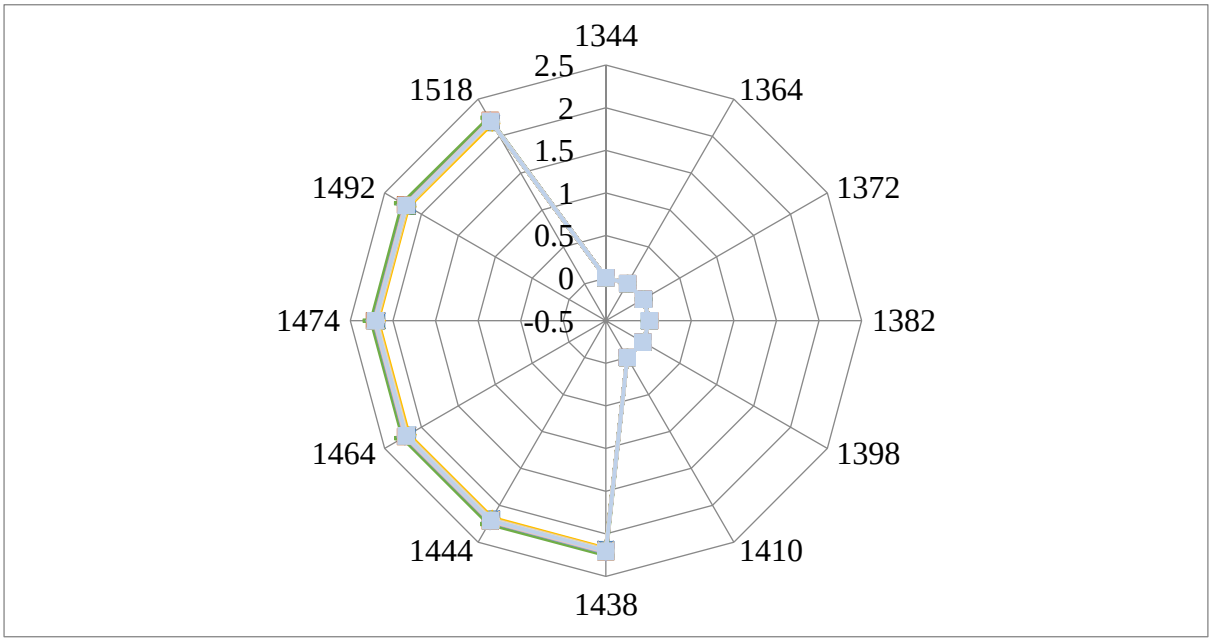

Figure 2 Aquagram for the lemon juice samples for range of water matrix coordinates

Aquaphotomics study for the lemon juice samples was performed. Spectra for the 12 activated water matrix coordinates (WAMACS) C1 to C12 in the region of water first overtone region (1300-1600nm) were studied for the samples under study. To understand the important wavelengths in the aquaphotomics range, correlation analysis between the aquaphotomics wavelength's absorbance and physicochemical parameters were studied. Correlational results for the same are presented in Fig3.

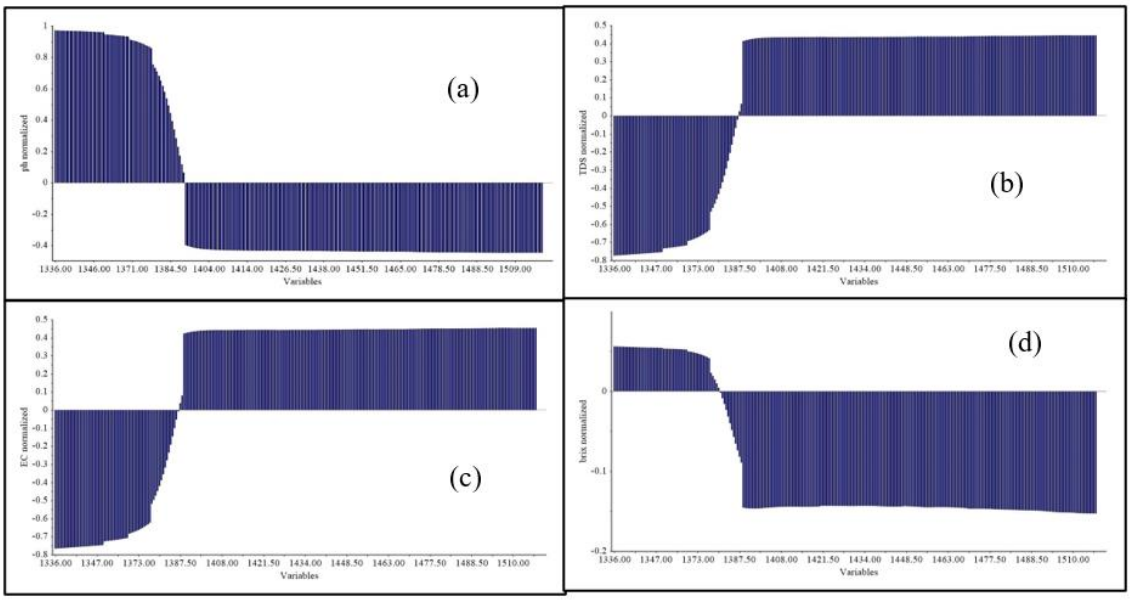

Figure 3 Correlation analysis for the absorbance of the aquaphotomics range with (a) pH, (b) TDS, (c) EC and (d) brix for the lemon juice samples.

Correlational analysis results revealed that the absorbance of the aquaphotomics wavelengths shows a high degree of positive corelation with pH values from 1336 to 1400 nm ($0.9 < r < 1$) and weak degree of negative correlation from 1400 – 1600nm ($r = -0.4$). Further with TDS the wavelengths showed strong negative correlation from 1336 – 1400nm ($-0.7 < r -0.8$) and weak positive relation from 1400 – 1600nm ($r = 0.4$). As EC and TDS are closely related to each other, thus the correlation between the aquaphotomics wavelengths and TDS was observed in similar fashion as of EC. Whereas the results of correlation of absorbance of the wavelengths under study had no or minimal correlation with the value of degree brix of the lemon juice samples.

The results of correlational analysis presented that the aquaphotomics wavelengths can be used to assess the pH, TDS and EC of the lemon juice samples and were not useful in measurement of the brix and RI of the samples under study.

The aquagrams and the correlation analysis helped in understanding that the properties of the lemon juice samples are affected by the changes in the water matrix coordinates from 1300-1600nm. The physicochemical properties are mostly affected by the v3 stretching of the water bond at 1344nm, water shell vibration at 1364 nm and 1382 nm, 1st and 3rd vibration at 1372 nm and free OH vibration at 1398nm.

Conclusion

The research work focusses on procuring the spectra and physicochemical parameters of 29 lemon juice samples. The results of physicochemical parameters showed that the pH value ranges from 1.6 to 2.2, TDS from 1939 to 2434 ppm, EC from 3.9 to 4.8 S/m, ˚Brix from 3 to 6 and RI from 1.33 to 1.346 for the collected lemon juice samples. Near infra spectra from 700-2500nm, showed that the absorbance was maximum from 900-2000nm and other spectral ranges are not important for quality analysis of lemon juice samples. As the aquaphotomics range is the sub set of 900-2000nm, thus further analysis were performed on selected range of 1344 to 1518 nm of water matrix coordinates. It was observed that 1438-1518 nm range was most important to understand the perturbation in the lemon juice samples. To study in depth,

correlational analysis were performed fro the selected aquaphototmics range, it was presented by the results that 1336 to 1400 nm have high coefficient of correlation (0.9<r<1) fro pH, EC and TDS of the lemon juice samples. Results present that the aquaphotomics range is very important to asses the quality of lemon juice samples.

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