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Color is many times related with the freshness of fruits and is also one of the most important fruit quality attributes because it is immediately perceived by the consumer. Unfortunately, undesirable color modifications can occur during fruit pasteurization processes. Changes in the color of cupuaçu fruit puree as the result of different intensity thermal treatments were mathematically modeled. Isothermal experiments were performed at 80°C, 90°C, 100°C, 110°C and 115°C for up to 120 minutes and color was measured by a tristimulus colorimeter using L (lightness), C (chroma) and h° (hue angle) CIE color space. When increasing time and/or temperature exposure, cupuaçu puree darkens (*i.e.* L decreases), gets a more vivid color (*i.e.* C slightly increases), and changes from a light yellow to a caramel like color (h° decreases). Total color difference (TCD), calculated as function of L, C and h° values, was the color parameter modeled. For each temperature, TCD increased along processing time following a power law model pattern ($TCD = a \times \text{time}^b$). The exponent *b*, was temperature dependent and was described by the Arrhenius law. One step non-linear regression to all data was carried out to estimate the model constants with its 95% confidence intervals. The parameters estimated values were $a=2.4$, $K_{100^\circ\text{C}}=0.4$ and $Ea=24.8 \text{ kJ/mol}$ with $R^2=0.98$. The results obtained are an useful tool to design pasteurization processes for minimizing puree color changes.

43-10

SELECTION OF OPTIMAL EXPERIMENTAL CONDITIONS FOR DETERMINING THE KINETICS OF SAFETY AND QUALITY INDICATORS IN PEA PUREE UNDER NON ISOTHERMAL CONDITIONS: A CASE STUDY

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The precision of estimates of kinetic parameters obtained with a regression of experimental data depends greatly on the experimental design. Selection of sampling times that minimize the confidence region of the regression is the basic concept of the so-called D-optimal design. This design was earlier applied to the Bigelow model, under non-isothermal conditions (linearly increasing temperature profile), for the estimation of the *z* and *Dr* values. It was shown that the optimum design greatly depends on the parameters themselves, on the heating rate and on the initial temperature. The objective of this work was to apply the D-optimal design for the estimation of *D*, and *z* for the thermal death of *Clostridium Botulinum* and for the loss of colour in pea puree. $D_{121.1}$ and *z* values of 0.21 min and 10 °C and 28.58 min and 42.87°C, for *Clostridium Botulinum* and colour, respectively, were considered. Initial temperatures from 50 to 90°C and heating rates from 2 to 12°C/min were analysed. Results showed that for *Clostridium Botulinum* the selection of optimal sampling times at any of the conditions tested would guarantee precise estimates. For the colour degradation, good estimates can be obtained for low initial temperatures and large heating rates while for the remaining conditions, optimal sampling times are not sufficient to obtain precise estimates, with precision decreasing up to 60% of its optimal value. It was concluded that because the kinetics of safety and quality indicators have a different sensitivity to temperature, their precise determination requires different experimental conditions.

44-1

WATER: SO COMMON, SO EXTRAORDINARY

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Three aspects of water will be covered in this presentation: the importance of water, unusual properties of water and their cause, and water-soluble interactions. Water is the most abundant substance on earth, the predominant component of biological matter and foods, the only substance on Earth that is present abundantly in all three physical states, the only inorganic substance that must be present in abundance to sustain life, and a major determinant of food perishability. Furthermore, water has highly unusual properties when compared to other molecules of similar weight and atomic composition. This is attributable to its unique structure which permits molecules to associate in three-dimensional, hydrogen-bonded networks. Association of water with solutes has a pronounced effect on solute behavior, and solutes, in turn, influence the structural arrangements assumed by water. It is odd, indeed, to find a substance so prevalent to behave so strangely, and to have this behavior go unnoticed by almost everybody!

44-2

POLYPHENOL CONTENT OF MALTS AND WORTS FROM BARLEYS, MILLETS AND SORGHUMS GERMINATED AT DIFFERENT TIMES AND TEMPERATURES

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In the brewing industry polyphenols contribute to haze in the product. There is

however, there is little information on polyphenol content in malts and worts from these grains. The purpose of this study was to evaluate the relationships of polyphenol content in grains to those in their malts and worts.

A total of 22 grains were placed in 5 groups which were: USA barley, Kenyan barleys, USA millets, Kenyan sorghums. Grains were germinated for 2, 4 and 6 days at temperatures of 14, 18, and 22°C and then kilned at 55°C for 18 hr to produce the malts. Malts were ground and mashed at 70°C for 60 min to produce the worts. Polyphenols were extracted from the grains and malts in methanol and the European Brewing Convention method 9.9.1 was used to measure polyphenol content in extracts and worts. All grains (22), malts (22 × 3 × 3) and worts (22 × 3 × 3) were analyzed for polyphenol content. The SAS General Linear Model was used for analysis of the 5 grain groups, 3 temperatures and 3 times of the malts and worts.

Mean grain polyphenol content in the 2 barley and 2 millet groups ranged from 0.43 to 0.64 % dry matter (%DM) which were all lower than the Kenyan sorghum 1.49 %DM ($p < 0.05$). The mean polyphenol content in the malts from the 2 barley and 2 millet groups ranged from 0.40 to 0.51 %DM which were all lower than the Kenyan sorghum group value of 1.30 %DM ($p < 0.05$). For malts, no significant differences ($p > 0.05$) for germination times and temperatures were found and no significant interactions were detected. For worts, both grain group and germination time had significant differences ($p < 0.05$). No significant interactions were present. Mean polyphenol content in worts from USA barley, USA millet, Kenyan barley and Kenyan sorghum ranged from 0.0057 to 0.0078 %DM which was lower ($p < 0.05$) than the polyphenol content in Kenyan millets of 0.0134 %DM. Polyphenol content at different germination times were all different from one another ($P < 0.05$) and values were 0.0060, 0.0073 and 0.0085 %DM for day 2, 4, and 6, respectively. Results indicate that the polyphenol content of the barleys, millets and sorghums groups used in this study ranged from 0.43 to 1.49 %DM and were similar on a group by group comparison to the malt polyphenol values. The mean polyphenol content of worts produced from all malt groups ranged from 0.0057 to 0.0134 %DM; but, the malt group with highest content (Kenyan sorghum) did not result in the wort with the highest value (Kenyan millet).

44-3

THIOSULFINATE PROFILES IN MODEL REACTION MIXTURES CONTAINING MIXED S-ALK(EN)YL-L-CYSTEINE SULFOXIDES AND ALLIINASE

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Alliinase (alliin alkyl sulfenate-lyase, EC 4.4.1.4) and S-alk(en)yl-L-cysteine sulfoxides (ACSO: methyl-, MeCSO; ethyl, EtCSO, *n*-propyl-, PrCSO, 1-propenyl-, 1-PeCSO; 2-propenyl- (allyl-), AlCSO) were either isolated from onion (*Allium cepa*) bulb tissue or synthesized. Alliinase and various combinations of ACSO (equimolar, total of 50 mM) were reacted in model systems containing 0.1 M Tris buffer (pH 7.5) at 21-23°C with the objective being to examine the fate of thioalk(en)yl groups. Reaction progress was followed by the evolution of pyruvate. Thiosulfinate ($R_2S(O)SR_2$) profiles were analyzed in dichloromethane extracts of the reaction mixtures using an HPLC procedure founded on gradient elution of 2-10% isopropanol in hexane and a silica column with detection at 254 nm. Quantification was based on extinction coefficients determined for pure, homologous thiosulfates prepared from a single ACSO.

About 72-94 mol% thioalk(en)yl residues derived from reacted ACSO appeared as thiosulfates in the reaction mixtures. Under the conditions used in the model reactions, the thiosulfate profile remained fairly constant over the 90-minute incubation period. However, the distribution between homologous ($R_2S(O)SR_2$) and heterologous ($R_1S(O)SR_2$ and $R_2SS(O)R_2$) thiosulfates varied greatly with the nature of the ACSO combinations subject to reaction with alliinase. For the various ACSO pairs evaluated, the molar distribution of thiosulfates formed were:

EtCSO/MeCSO: EtS(O)SEt : EtS(O)SMe : EtSS(O)Me : MeS(O)SMe = 3:2:2:1;
PrCSO/EtCSO: PrS(O)SPr : PrS(O)SEt : PrSS(O)Et : EtS(O)SEt = 11:3:4:1;
PrCSO/MeCSO: PrS(O)SPr : PrS(O)SMe : PrSS(O)Me : MeS(O)SMe = 15:2:3:tr;
AlCSO/MeCSO: AlIS(O)SAl : AlIS(O)SMe : AlISS(O)Me : MeS(O)SMe = 23:1:2:tr;
AlCSO/EtCSO: AlIS(O)SAl : AlIS(O)SEt : AlISS(O)Et : EtS(O)SEt = 14:1:2:tr;

These results were modeled in terms of reaction selectivity of alliinase on the ACSO species present, and the relative reactivity of the initial (transient) product of the enzyme reaction, the sulfenic acids (RSOH), involved in homologous and heterologous condensation reactions. The fate and control of these organosulfur compounds is relevant to flavor quality and pungency in selected food systems.

44-4

THE EFFECT OF OZONE AND OXYGEN EXPOSURE ON THE DEGRADATION KINETICS OF ALL-TRANS β -CAROTENE, 9-CIS β -CAROTENE, β -CRYPTOXANTHIN, AND LYCOPENE

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Carotenoids are important food constituents because of their role as natural colorants, precursors to vitamin A, and ability to prevent peroxidation processes. These pigments protect against the harmful effects of oxidizing conditions in foods such as exposure to light, air and photosensitizers. However, their highly unsaturated polyene chain of conjugated double bonds confer susceptibility to oxidative degradation. Ozone is an ubiquitous atmospheric substance which can be used to decrease micro-