Oriental Tobacco

Oriental Tobacco : Unburnt Chemistry & Toxicity

Potentiometric stripping analysis of zinc, cadmium and lead in tobacco leaves (Nicotiana tabacum L.) and soil samples By Kalicanin, Biljana; Velimirovic, Dragan From International Journal of Electrochemical Science (2012), 7(1), 313-323. Language: English, Database: CAPLUS

The potentiometric stripping anal. (PSA) with oxygen as the oxidant has been used to det. total zinc, cadmium and lead levels in tobacco leaves (Nicotiana tabacum L.), agricultural soil and cigarettes. The content of these metals in the leaves of the analyzed tobacco cultivars (Virginia, Burley and Oriental), obtained from locations which were close to industrial facilities and main roads, was higher than in the tobacco which was grown in rural areas. In addn. to the cited potential sources of Zn, Cd and Pb, what also has an effect on the content of these metals in the studied samples of tobacco leaves is the soil in which the tobacco plant is cultivated. Thus the content of zinc in the tobacco leaves of all the studied tobacco plant types was approx. five times, of cadmium was approx. two times and lead approx. three times smaller than the content in the soil samples taken from the studied areas. The total content of heavy metals in fine brand of cigarettes was lower than in popular brand of cigarettes. The results of this work suggest that PSA may be a good method for zinc, cadmium and lead detn. in soil, tobacco leaves as well as in different plant species.

Ultrasound-assisted extraction of total phenols and flavonoids from dry tobacco (Nicotiana tabacum) leaves By Karabegovic, Ivana T.; Veljkovic, Vlada B.; Lazic, Miodrag L. From Natural Product Communications (2011), 6(12), 1855-1856. Language: English, Database: CAPLUS

Yields of extd. substances, as well as total phenol and flavonoid compds. obtained by classical and ultrasonic extns. from dry leaves of two tobacco types (oriental and Virginia) by two different solvents (acetone and methanol) at two operating temps. (25 and 40°C) were compared. The yield of extractive, as well as total phenol and flavonoid compds. depended on the type of solvent, operational temp. and the tobacco type. The importance of these factors was assessed using 24 full factorial expts. without replication.

Analysis of certain nitrogenous compounds in tobacco. Part 1: adenosine, 2,5- and 2,6-deoxy-fructosazines, mannosamine and glucosamine By Moldoveanu, Serban C.; Byrd, Crystal H.; Gerardi, Anthony R. From Beitraege zur Tabakforschung International (2011), 24(5), 233-242. Language: English, Database: CAPLUS

Nitrogenous compds. such as amino acids and proteins are frequently analyzed in tobacco since they are considered precursors of toxicants in cigarette smoke. However, much less

attention is given to other nitrogenous compds. such as amino sugars and deoxyfructosazines, although their concn. in tobacco can be equal to or even higher than that of most free amino acids. These nitrogenous compds. may contribute to the formation of toxicants in smoke, or may contribute to the sensory properties of cigarette smoke, reasons for which their anal. is important. This study describes a procedure for the anal. of adenosine, 2,5- and 2,6-deoxyfructosazines (DFs), mannosamine and glucosamine in tobacco. The anal. uses a liq. chromatog.-tandem mass spectrometry (LC/MS/MS) technique. Sample prepn. for anal. consists of the extn. of the tobacco with a soln. of 90% water and 10% methanol, followed by filtration. The sepn. of the analytes was done on a hydrophilic interaction liq. chromatog. HILIC column using an isocratic procedure with a solvent consisting of 78% CH3CN, 22% H2O, that also contained 0.1% HCOOH and 0.143 g/L CH3COONH4. The measurements were done using electrospray pos. ionization mass spectrometric detection. The anal. procedure was validated and was proven very reliable. A no. of tobaccos were analyzed, including several flue-cured and Burley USA tobaccos, off-shore tobaccos, two Oriental tobaccos, two green tobaccos, as well as tobaccos from com. and Kentucky ref. cigarettes. The ranges for the analytes per g tobacco were found between 0.4 and 20.3 μg/g for adenosine, between 0.0 and 608.5 μg/g for 2,5-DF, between 0.0 and 424.5 μg/g for 2,6-DF, between 12.5 and 415.5 μg/g for mannosamine and between 25.9 and 1885.7 μg/g for glucosamine. The study also indicated that the levels of DFs and that of the amino sugars in tobacco show a very good correlation. This correlation can be explained by the same source of the two classes of compds., namely the reaction of (reducing) sugars and ammonia.

Method development for the determination of 52 pesticides in tobacco by liquid chromatography-tandem mass spectrometry By Mayer-Helm, Bernhard From Journal of Chromatography, A (2009), 1216(51), 8953-8959. Language: English, Database: CAPLUS, DOI:10.1016/j.chroma.2009.10.077

A method using reversed phase liq. chromatog.-electrospray ionization-tandem mass spectrometry was developed for the detn. of 52 pesticides in tobacco. The influence of mobile phase additives was investigated to improve sensitivity and accuracy of the method and to reduce matrix effects. The tobacco exts. were purified via a Chem Elut partition cartridge by consecutive elution with pentane followed by dichloromethane. The two fractions were further purified by Florisil solid-phase extn. with acetone or di-Et ether elution. An addnl. dispersive solid-phase extn. step with primary-secondary amine led to decreased recoveries of several pesticides due to degrdn. or binding to the sorbent. The method was validated for the tobacco types Burley, Oriental and Virginia. The recovery rates of almost all pesticides ranged between 70 and 120%. The limits of quantification were below or near the 10 ng/g level. Few but significant differences between the tobacco types could be found regarding recovery and sensitivity.

Heavy-metal concentration in tobacco leaves in relation to their available soil fractions By Golia, E. E.; Dimirkou, A.; Mitsios, I. K. From Communications in Soil Science and Plant Analysis (2009), 40(1-6), 106-120. Language: English, Database: CAPLUS, DOI:10.1080/00103620802623570

Tobacco (Nicotiana tabacum) is one of the most important agricultural products in Greece. The accumulation of heavy metals in tobacco leaves in accordance with a possible risk of transferring them to people by smoke is well known. To monitoring heavy-metal contents in soils, as well as in tobacco leaves, a 6-yr survey was conducted in the Thessaly region (central Greece). The concn. of zinc (Zn), copper (Cu), nickel (Ni), cadmium (Cd), iron (Fe), and manganese (Mn) was measured both in soils and in air-cured (Burley), flue-cured (Virginia), and sun-cured (Oriental-filling) tobacco leaves in lower and upper leaves (primings). Regression anal. was conducted between soil and tobacco heavy-metal content to examine the possibility of predicting tobacco heavy-metal levels based on the results of soil anal. DTPA-extractable levels. The results showed a high correlation between Oriental tobacco heavy-metal content and DTPA-extd. heavy-metal level in soils. Although regressions based on the pooled data from the three tobacco types adequately predicted tobacco heavy-metal levels, better fits were obtained when regression models were used for Oriental tobacco sep. Statistically significant neg. correlations were recorded between heavy-metal concns. in Oriental tobacco leaves and soil pH, in all primings. Therefore, low soil pH value leads to an increased availability of heavy metals in tobacco leaves.

Arsenic Concentration in Tobacco Leaves: A Study on Three Commercially Important Tobacco (Nicotiana tabacum L.) Types By Lugon-Moulin, Nicolas; Martin, Florian; Krauss, Marc R.; Ramey, Patrice B.; Rossi, Luca From Water, Air, & Soil Pollution (2008), 192(1-4), 315-319. Language: English, Database: CAPLUS, DOI:10.1007/s11270-008-9658-3

In recent years, arsenic (As) has received increased attention as humans may be exposed to it through occupational and environmental exposure. Tobacco (Nicotiana tabacum L.) like other crops can uptake this element from the soil, which may lead to human exposure. Here, we report on a survey on arsenic in cured or processed tobacco leaves obtained from Africa, Asia, Europe, South and North America. A total of 1,431 leaf samples of flue-cured, burley, and Oriental tobaccos were obtained from various sampling locations during 2002 to 2004. Arsenic concn. in the samples averaged 0.4 ± 0.6 μg g-1 as detd. by inductively coupled plasma-mass spectrometry. Recorded values from most samples showed that concns. of arsenic were usually found at the lower end of the distribution. Significant differences were found among tobacco types, sampling locations, and crop years. Arsenic concns. were rather low in the majority of regions investigated, which is compatible with data from the literature. However, sample size was small and sampling geog. restricted. Our results would need to be validated with a larger dataset.

Comparative study of pesticide multi-residue extraction in tobacco for gas chromatography-triple quadrupole mass spectrometry By Lee, Jeong-Min; Park, Jin-Won; Jang, Gi-Chul; Hwang, Keon-Joong From Journal of Chromatography, A (2008), 1187(1-2), 25-33. Language: English, Database: CAPLUS, DOI:10.1016/j.chroma.2008.02.035

This study was performed to select a rapid and accurate sample prepn. method for tobacco and to apply gas chromatog.-triple quadrupole mass spectrometry (GC-MS/MS) to the highly selective and sensitive detection of pesticides. Three sample prepn. methods, including the conventional liq.-liq. extn. (LLE), pressurized liq. extn. (PLE), and QuEChERS (quick, easy, cheap, effective, rugged and safe) methods were compared for tobacco. These methods were validated for 49 pesticides that are in the CORESTA Agrochem. Advisory Committee guide and that are amenable to GC-MS/MS detn. LLE with acetonitrile and PLE with acetone were followed by solid-phase extn. (SPE) and anal. by GC-MS/MS. In the QuEChERS method, the effects of sorbents, such as primary secondary amine (PSA), octadecylsilane (C18) and graphitized carbon black (GCB), and matrix of the analytes in 3 tobacco types - flue-cured, burley and oriental - were investigated. MS/MS acquisition provided high specificity and selectivity for pesticides and a low limit of detection and quantification. QuEChERS by using PSA alone and the matrix-matched stds. gave good recoveries and RSD values for the three types of tobacco. The method yielded higher and more consistent recoveries of these analytes than LLE and PLE. The QuEChERS method needed no complex clean-up procedure and could be used as an alternative to LLE and PLE methods for rapid and sensitive detn. of pesticides.

Enantiomeric analysis of anatabine, nornicotine and anabasine in commercial tobacco by multi-dimensional gas chromatography and mass spectrometry By Liu, Baizhan; Chen, Chaoying; Wu, Da; Su, Qingde From Journal of Chromatography, B: Analytical Technologies in the Biomedical and Life Sciences (2008), 865(1-2), 13-17. Language: English, Database: CAPLUS, DOI:10.1016/j.jchromb.2008.01.034

A fully automated multi-dimensional gas chromatog. (MDGC) system with a megabore precolumn and cyclodextrin-based anal. column was developed to analyze the enantiomeric compns. of anatabine, nornicotine and anabasine in com. tobacco. The enantiomer abundances of anatabine and nornicotine varied among different tobacco. S-(-)-anatabine, as a proportion of total anatabine, was 86.6% for flue-cured, 86.0% for burley and 77.5% for oriental tobacco. S-(-)-nornicotine, as a proportion of total nornicotine, was 90.8% in oriental tobacco and higher than in burley (69.4%) and flue-cured (58.7%) tobacco. S-(-)-anabasine, as a proportion of total anabasine, was relatively const. for flue-cured (60.1%), burley (65.1%) and oriental (61.7%) tobacco. A simple solvent extn. with dichloromethane followed by derivatization with trifluoroacetic anhydride gave relative std. deviations of less than 1.5% for the detn. of the S-(-)-isomers of all three alkaloids. The study also indicated that, a higher proportion of S-(-)-nornicotine is related to the more active nicotine demethylation in the leaf.

Determination of volatile organic acids in oriental tobacco by needle-based derivatization headspace liquid-phase microextraction coupled to gas chromatography/mass spectrometry By Sun, Shi-Hao; Xie, Jian-Ping; Xie, Fu-Wei; Zong, Yong-Li From Journal of Chromatography, A (2008), 1179(2), 89-95. Language: English, Database: CAPLUS, DOI:10.1016/j.chroma.2007.11.102

A method coupling needle-based derivatization headspace liq.-phase microextn. with gas chromatog.-mass spectrometry (HS-LPME/GC-MS) was developed to det. volatile org. acids in tobacco. The mixt. of N,O-bis(trimethylsilyl)trifluoroacetamide and decane was utilized as the solvent for HS-LPME, resulting that extn. and derivatization were simultaneously completed in one step. The solvent served two purposes. First, it pre-concd. volatile org. acids in the headspace of tobacco sample. Second, the volatile org. acids extd. were derivatized to form silyl derivs. in the drop. The main parameters affecting needle-based derivatization HS-LPME procedure such as extn. and derivatization reagent, microdrop vol., extn. and derivatization time, and preheating temp. and preheating time were optimized. The std. addn. approach was essential to obtain accurate measurements by minimizing matrix effects. Good linearity ($R2 \geq 0.9804$) and good repeatability (RSDs ≤ 15.3%, n = 5) for 16 analytes in spiked std. analytes sample were achieved. The method has the addnl. advantages that at the same time it is simple, fast, effective, sensitive, selective, and provides an overall profile of volatile org. acids in the oriental tobacco. This paper does offer an alternative approach to det. volatile org. acids in tobacco.

Free and Conjugated Phytosterols in Cured Tobacco Leaves: Influence of Genotype, Growing Region, and Stalk Position By Liu, Wen-Hui; Yong, Guo-Ping; Fang, Li; Wang, Shao-Kun; Bai, Hai-Jun; Jiang, Jia-He; Liu, Shao-Min From Journal of Agricultural and Food Chemistry (2008), 56(1), 185-189. Language: English, Database: CAPLUS, DOI:10.1021/jf0722708

Although phytosterols in tobacco leaves have specific effects on tobacco quality, there is little research on the distribution of free and conjugated phytosterols in various tobacco leaves. In this paper, we explored the content and compn. of phytosterols in representative cured tobacco leaves by gas chromatog. of TMS-ether derivs. We found that phytosterol contents in tobacco leaves ranged from 1.0 to 2.5 mg/g of dried leaf tissue, depending on different types of tobacco leaves. The majority of phytosterols (75-85%) were conjugated as ester and glycosides, with only about 15-25% existing in the free form. Furthermore, the genetic variability gives rise to the significant differences among different tobacco types with phytosterol levels: the contents of phytosterols in tobacco leaves decreased in the order of flue-cured tobacco, Oriental tobacco, Burley tobacco, cigar tobacco, and Maryland tobacco. At the same time, the tobacco curing process leads to a difference in phytosterol existing-form distribution in some variation laws.

Thermal desorption/pyrolysis coupled with photoionization time-of-flight mass spectrometry for the analysis and discrimination of pure tobacco samples By Streibel, T.; Mitschke, S.; Adam, T.;

Weh, J.; Zimmermann, R. From Journal of Analytical and Applied Pyrolysis (2007), 79(1-2), 24-32. Language: English, Database: CAPLUS, DOI:10.1016/j.jaap.2006.12.017

Three different tobacco samples (Burley, Virginia, and Oriental) were thermally desorbed at varying temps. (190, 250, and 310°) and the evolved gas phase at every temp. step was analyzed applying single photon ionization (SPI)-time-of-flight mass spectrometry (TOFMS) and resonance enhanced multiphoton ionization (REMPI)-time-of-flight mass spectrometry. These soft and selective ionization techniques allow fast and comprehensive online monitoring of a large variety of aliph. and arom. substances with almost no fragmentation of mol. ions. Many oxygen-contg. compds. could be detected such as phenol, hydroquinone, and (vinyl)guiacol along with unsatd. hydrocarbons and nicotine. In addn., with REMPI, a large variety of PAH were accessible. Different tobacco types yield slightly distinguished mass spectra. By utilizing statistical tools (Fisher criterion and PCA) the 3 tobaccos can be discerned rather rapidly from each other and possible marker compds. for a given tobacco can be identified. Extension of this newly conceived method to other biomass material and potential coupling to other methods of thermal anal. seems feasible in the future.

Rapid quantification of sucrose esters in oriental tobacco by liquid chromatography-ion trap mass spectrometry By Ding, Li; Xie, Fuwei; Zhao, Mingyue; Wang, Sheng; Xie, Jianping; Xu, Guowang From Journal of Separation Science (2007), 30(1), 35-41. Language: English, Database: CAPLUS, DOI:10.1002/jssc.200600270

A rapid and sensitive LC-MS/MS method was developed for the quant. detn. of sucrose esters (SEs) in Oriental tobacco samples. The sample prepn. involved a 10-min sonication extn. procedure with acetone and 5-fold diln. of the ext. with methanol. The expt. was carried out in pos. ion mode by ESI IT mass spectrometer. Because of lack of authentic stds. of SEs, sucrose octaacetate (internal std., IS) was used as a surrogate to validate the proposed method. Matrix-matched std. calibration was used for quantification of IS in the spiked samples. Under optimized MS/MS conditions, an LOQ of 3.9 μg/g was achieved for IS, with an LOD of about 1.2 μg/g. Recoveries for IS were 95-97%. Among 19 monitored SEs, the contents of 11 SEs had RSDs lower than 13.7%. The method, with very little sample handling and good sensitivity, was applied to the rapid quantification of SEs in 4 Oriental tobacco samples. It appears that the sum of contents of the 5 SEs with MW 650, 664, and 678 Da occupied approx. 80% of the total content of SEs.

Determination of trace metals by ICP-OES in plant materials after preconcentration of 1,10-phenanthroline complexes on activated carbon By Mikula, Barbara; Puzio, Bozena From Talanta (2007), 71(1), 136-140. Language: English, Database: CAPLUS, DOI:10.1016/j.talanta.2006.03.041

In this work, 1,10-phenanthroline was used as a complexing agent for the sepn. and preconcn. of Cd(II), Co(II), Ni(II), Cu(II) and Pb(II) on activated carbon. The metals were adsorbed on

activated carbon by two methods: static (1) and dynamic (2). The optimal condition for sepn. and quant. preconcn. of metal ions with activated carbon for the proposed methods was for (1) in the static methods in the pH range 7-9. The desorption was found quant. with 8 mol dm-3 HNO3 for Cd(II) (92.6%), Co(II) (95.6%), Pb(II) (91.0%), and with 3 mol dm-3 HNO3 for Cd(II) (95.4%), Pb(II) (100.2%). The preconcn. factor was 100 with R.S.D. values between 1.0 and 2.9%. For (2), the dynamic method (SPE), the pH range for the quant. sorption was 7-9. The desorption was found quant. with 8 mol dm-3 HNO3 for Cd(II) (100.6%), Pb(II) (94.4%), and reasonably high recovery for Co(II) (83%), Cu(II) (88%). The optimum flow rate of metal ions soln. for quant. sorption of metals with 1,10-phenanthroline was 1-2 cm3 min-1 whereas for desorption it was 1 cm3 min-1. The preconcn. factor was 50 for all the ions of the metals with R.S.D. values between 2.9 and 9.8%. The samples of the activated carbon with the adsorbed trace metals can be detd. by ICP-OES after mineralization by a high-pressure microwave mineralizer. The proposed method provides recovery for Cd (100.8%), Co (97.2%), Cu (94.6%), Ni (99.6%) and Pb (100.0%) with R.S.D. values between 1.2 and 3.2%. The preconcn. procedure showed a linear calibration curve within the concn. range 0.1-1.5 μg cm-3. The limits of detection values (defined as "blank + 3s" where s is std. deviation of the blank detn.) are 5.8, 70.8, 6.7, 24.6, and 10.8 μg dm-3 for Cd(II), Pb(II), Co(II), Ni(II) and Cu(II), resp., and corresponding limit of quantification (blank + 10s) values were 13.5, 151.3, 20.0, 58.9 and 33.2 μg dm-3, resp. As a result, these simple methods were applied for the detn. of the above-mentioned metals in ref. materials and in samples of plant material.

Rapid characterization of the sucrose esters from oriental tobacco using liquid chromatography/ion trap mass spectrometry By Ding, Li; Xie, Fuwei; Zhao, Mingyue; Xie, Jianping; Xu, Guowang From Rapid Communications in Mass Spectrometry (2006), 20(19), 2816-2822. Language: English, Database: CAPLUS, DOI:10.1002/rcm.2664

Sucrose esters (SEs) from oriental tobacco are normally characterized by gas chromatog./mass spectrometry (GC/MS) after a long sapon. and derivatization procedure. To simplify the process, a rapid method has been developed by using liq. chromatog. coupled with electro-spray ion trap mass spectrometry (LC/ESI-MSn). Using the characteristic fragmentation behavior of abundant SEs identified by GC/MS after purifn. by gel permeation chromatog. (GPC) from cuticular waxes of green oriental tobacco leaf, two types of SEs from green and cured oriental tobacco were identified by MSn anal. The first is one of three types reported formerly and has 13 SE homologs. However, the presence of unsatn. in one of the acyl substituents of this first type gave rise to a new series with three homologs. The other was a new type and had three homologs. The proposed method enables the rapid and sensitive characterization of SEs from oriental tobacco.

Cadmium concentration in tobacco (Nicotiana tabacum L.) from different countries and its relationship with other elements By Lugon-Moulin, Nicolas; Martin, Florian; Krauss, Marc R.; Ramey, Patrice B.; Rossi, Luca From Chemosphere (2006), 63(7), 1074-1086. Language: English, Database: CAPLUS, DOI:10.1016/j.chemosphere.2005.09.005

Cadmium accumulation in crop plants, such as tobacco (N. tabacum L.), can lead to human exposure to this carcinogenic metal. To better define actual Cd distribution in cured or processed tobacco leaves from chief tobacco-producing regions, the authors analyzed 755 leaf samples of 3 major types (Flue-cured, Burley, and Oriental) obtained from 13 countries during 2001-2003. This survey may help identify regions with low- or high-Cd concns. in tobacco to obtain insight into the cause of the concn. extremes and to assist in defining strategies to reduce Cd in tobacco. Cadmium concns. in the samples ranged from 0 to 6.78 μg g-1, as detd. by ICP-MS. Significant differences were found among types and among countries, but significant interactions between type and country were found. Variations in Cd concns. were also found in all countries. The results suggest an important contribution of the field (e.g., bioavailable Cd in soil, other soil characteristics) to the Cd concn. in tobacco. Finally, the correlation between the concn. of Cd and that of other elements differed among the types, which could be effectively discriminated based on the concns. of 20 elements.

Characterization of Cigarette Tobacco by Direct Electrospray Ionization-Ion Trap Mass Spectrometry (ESI-ITMS) Analysis of the Aqueous Extract-A Novel and Simple Approach By Ng, Lay-Keow; Lafontaine, Pierre; Vanier, Micheline From Journal of Agricultural and Food Chemistry (2004), 52(24), 7251-7257. Language: English, Database: CAPLUS, DOI:10.1021/jf040203x

In support of the efforts to combat smuggling, as well as illegal sale and distribution of cigarettes, an anal. approach for the characterization of tobacco has been proposed and evaluated. It involves aq. extn. of the filler tobaccos followed by direct anal. of the exts. by electrospray ionization-ion trap mass spectrometry (ESI-ITMS) in the neg. mode. Typically, the deprotonated ions, [M - H]-, of org. acids (malic, citric, caffeic, quinic acid) and polyphenols (chlorogenic acid, rutin, scopoletin) were detected. MS/MS spectra of the ion at m/z 191, which is the [M - H]- of quinic acid, citric acid, and scopoletin, and a fragment ion of chlorogenic acid were acquired. Significant differences in the MS and MS/MS spectra were obsd. between counterfeit samples and the corresponding authentic brand name cigarettes. Anal. of 25 com. cigarettes showed that straight Virginia blends were readily distinguished from the blended products contg. different tobacco types (Virginia, burley, and Oriental). The former exhibited consistently higher relative abundances of m/z 353 (chlorogenic acid) to m/z 133 (malic acid) in the MS spectra (0.9-1.2 vs. 0.4-0.6) and higher intensity ratios of m/z 176 (scopoletin) to m/z 173 (0.4-0.8 vs. 0.1-0.3) and of m/z 127 (quinic acid) to m/z 173 (0.7-1.0 vs. 0.3-0.5) in the MS/MS spectra. Evidence is presented to demonstrate that the spectral differences were related not only to the tobacco type (Virginia, burley and Oriental) but also to the tobacco part (stem, lamina) used in the manuf. of the cigarettes.

Formation of Nitric Oxide during Tobacco Oxidation By Im, Hoongsun; Rasouli, Firooz; Hajaligol, Mohammad From Journal of Agricultural and Food Chemistry (2003), 51(25), 7366-7372. Language: English, Database: CAPLUS, DOI:10.1021/jf030393w

The sources of NO during biomass oxidn., and in particular tobacco oxidn., have been disputed. Literature results range from decompn. of nitrate to the oxidn. of atm. nitrogen. To rectify these discrepancies, this study focuses on the sources of nitric oxide during the oxidn. of tobacco samples. When Burley tobacco was heated in a partial oxygen atm., NO was produced at two distinct temp. ranges, namely 275-375° (the low-temp. range) and 425-525° (the high-temp. range). The formation of NO in the low-temp. range with Burley tobacco was found to be unaffected by oxygen, while the formation of NO in the high-temp. range required an oxygen atm. With Bright and Oriental tobacco, NO was produced only within the higher-temp. range. To understand the formation processes and the sources of NO formation within these two temp. ranges, several endogenous nitrogenous tobacco compds. were examd. These were mixed with non-nitrogenous biomass model materials, namely cellulose, pectin, xylan, or lignin, which also occur naturally in tobacco, and the mixts. were heated in a flow tube reactor under a partially oxidative atm. A com. gas analyzer was used to monitor the formation of NO during heating. Nitrate ion was detd. to be the source of NO formation in the range of 275-375°. This ion was decompd. in a carbonaceous surrounding to produce NO. For NO formation at the higher temp. range, amino acids and proteins were shown to be the sources. The interaction between nitrogenous org. compds. (amino acids and proteins) and pectin first produced a nitrogen-contg. char at a temp. below 350°. Oxidn. of this char at the higher temps. produced NO.

Characterizing biomatrix materials using pyrolysis molecular beam mass spectrometer and pattern recognition By Shin, Eun-Jae; Hajaligol, Mohammad R.; Rasouli, Firooz From Journal of Analytical and Applied Pyrolysis (2003), 68-69, 213-229. Language: English, Database: CAPLUS, DOI:10.1016/S0165-2370(03)00079-2

Fingerprinting techniques have been applied to pyrolysis mol. beam mass spectra of a complex biomatix material such as tobacco. Pyrolysis products of three major tobaccos (burley, bright and oriental) and their blends were scanned from m/z 25 to 500 by a mol. beam mass spectrometer (MBMS) in high vacuum and soft ionization (25 eV). The resultant complex mass spectra were further analyzed using multivariate data anal. (pattern recognition) to discover the underlying chem. differences that may not be obvious by comparison of such complex mass spectra. Using the MBMS and pattern recognition techniques, we were able to statistically distinguish among different major tobaccos and their blends and show their characteristic nitrogen contg. products, oriental by its abundant carbohydrate-derived products and bright by its intermediate behavior. Blended tobacco samples of burley and oriental with a ratio of 66:34 resulted in similar product compn. to that of bright. Classes of pyrolysis products of a tobacco sample at different reaction conditions were also extd. by using the same anal. These results indicate that this approach could be used to rapidly predict biomass pyrolysis product distribution.

Application of pattern recognition method for color assessment of oriental tobacco based on HPLC of polyphenols By Dagnon, S.; Edreva, A. From Beitraege zur Tabakforschung International (2003), 20(5), 355-359. Language: English, Database: CAPLUS

The color of Oriental tobaccos was organoleptically assayed, and HPLC of polyphenols was performed. The major tobacco polyphenols (chlorogenic acid, its isomers, and rutin), as well as scopoletin and kaempferol-3-rutinoside were quantified. HPLC polyphenol profiles were processed by pattern recognition method (PRM), and the values of indexes of similarity (Is,%) between the cultivars studied were detd. It was shown that data from organoleptic color assessment and from PRM based on HPLC profiles of polyphenols of the cultivars studied are largely compatible. Hence, PRM can be suggested as an addnl. tool for objective color evaluation and classification of Oriental tobacco.

Leaf chemistry: basic chemical constituents of tobacco leaf and differences among tobacco types By Leffingwell, J. C. Edited By:Davis, Daniel Layten; Nielsen, Mark T From Tobacco: Production, Chemistry and Technology (1999), 265-284. Language: English, Database: CAPLUS

A review with 59 refs. concerning the known compn. and chem. of tobacco types that impact tobacco quality and differentiate tobacco types. Emphasis is given on major tobacco types utilized com., i.e., Virginia (flue-cured), air-cured (Burley and cigar) and Oriental.

Determination of volatile acids in tobacco, tea, and coffee using derivatization-purge and trap gas chromatography-selected ion monitoring mass spectrometry By Clark, T. Jeffrey; Bunch, John E. From Journal of Chromatographic Science (1997), 35(5), 206-208. Language: English, Database: CAPLUS

Short-chain acids from agricultural products are simultaneously extd. and derivatized using methanolic hydrochloric acid. Acetic, isobutyric, butyric, isovaleric, valeric, hexanoic, 3-methylvaleric, heptanoic, and nonanoic acids are quantitated using purge and tap gas chromatog. with selected ion monitoring mode mass spectrometry. Flue-cured, burley, and oriental tobacco varieties are compared based on their volatile org. acid content. Com. coffee, tea, and three cigarette brands are analyzed, and their differences are evaluated to demonstrate the utility of this technique for natural product anal.

Determination of free amino acids in tobacco by HPLC with fluorescence detection and precolumn derivatization By Yang, S. S.; Smetena, I. From Chromatographia (1993), 37(11-12), 593-8. Language: English, Database: CAPLUS, DOI:10.1007/BF02274107

An HPLC method for the detn. of primary amino acids in tobacco, based on precolumn derivatization with the fluorogenic reagent naphthalene-2,3-dicarboxaldehyde, is described. Sample prepn. consists of a single step of extn. with water-ethanol (1:1, vol./vol.) at ambient temp. (assisted by sonication), followed by filtration of an aliquot and addn. of derivatization reagents. High performance liq. chromatog. sepn. of the derivatized amino acids is performed

on a Novapak C-18 column using fluorescence detection with excitation and emission wavelengths set at 246 and 470 nm resp. Extn. efficiency, matrix interferences and other important variables are studied. This method has been used to analyze different types of tobaccos including burley, bright and oriental with satisfactory results.

Assessment of major carcinogens and alkaloids in the tobacco and mainstream smoke of USSR cigarettes By Djordjevic, Mirjana V.; Sigountos, Claire W.; Hoffmann, Dietrich; Brunnemann, Klaus D.; Kagan, Mark R.; Bush, Lowell P.; Safaev, R. D.; Belitskii, G. A.; Zaridze, D. From International Journal of Cancer (1991), 47(3), 348-51. Language: English, Database: CAPLUS, DOI:10.1002/ijc.2910470306

Tobacco and mainstream smoke of USSR cigarettes were analyzed for carcinogens. The pH values of suspensions of the tobacco (5.4-5.6) and the nitrate content of the tobaccos (0.4-1.7%) were as expected for flue-cured and sun-cured tobaccos and mixts. thereof. The nicotine levels of the cigarette tobaccos (0.76-0.94%) and total alkaloid content (0.85-1.08%) were relatively low compared with tobaccos used in Western European and US cigarettes. The concns. of tobacco-specific N-nitrosamines in the cigarette tobaccos were also low (N'-nitrosonornicotine 0.36-0.85 μg/g) compared with those in bright, oriental and blended cigarette tobaccos in Western countries (0.3-19 μg/g). The 2 nonfilter and 4 filter cigarettes from the USSR had slow burning rates and yielded 14.0-16.7 puffs/cigarette, while puff yields for com. cigarettes in Western countries av. ≤11 puffs/cigarette. Consequently, tar and benzo[a]pyrene yields in the smoke of all cigarettes as well as nitrosamine yields were high, esp. in the smoke of the filter cigarettes. It appears that an increase in the burning rates of these cigarettes should lead to lower smoke yields.

Performed tobacco-specific nitrosamines in tobacco-role of nitrate and influence of tobacco type By Fischer, Sophia; Spiegelhalder, Bertold; Preussmann, Rudolf From Carcinogenesis (1989), 10(8), 1511-17. Language: English, Database: CAPLUS

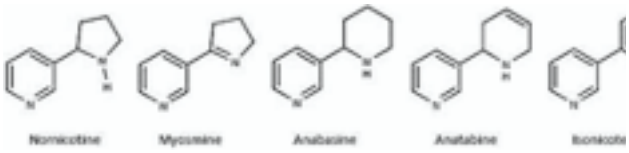
Fifty-five types of com. cigarettes on the open market in the Federal Republic of Germany and several samples of pure tobacco types were analyzed for preformed tobacco-specific nitrosamines (TSNA) and nitrate in the tobacco. For the cigarette tobaccos the obsd. range for N'-nitrosonornicotine (NNN) was 50-5316 ng/cigarette and for 4-(methylnitrosamino)-1-(3-pyridyl)-1-butanone (NNK) from not detected (<50 ng/cigarette) to 1120 (ng/cigarette). Nitrate levels ranged from 0.6 to 14.4 mg/cigarette. The highest TSNA values were obtained for cigarettes made of dark tobaccos and the lowest for Oriental type cigarettes. There is a correlation between TSNA and nitrate levels. The tobacco type is another important influencing factor, esp. for NNK. In Virginia tobaccos unexpectedly high NNK values were obsd. For the samples of the pure tobacco types, NNN levels ranged from 20 to 8850 ppb and NNK levels from not detected (<50 ppb) to 1400 ppb. The obsd. range for nitrate was from traces (<0.005%) to 4.1%. Pure Oriental tobaccos which are low in nitrate showed the lowest TSNA concns. In the high nitrate Burley tobaccos the highest TSNA

concns. could be detd. Virginia tobaccos which show a low nitrate content and low in NNN but rather high NNK concns. were found. The results from these pure tobacco types demonstrate that the nitrate content of the tobacco has a great influence on the TSNA level. However, Virginia tobaccos show higher NNK concns. than expected according to their low nitrate content.

Solid-state 15N NMR studies of tobacco leaves By Ma Zhiru; Barich Dewey H; Solum Mark S; Pugmire Ronald J From Journal of agricultural and food chemistry (2004), 52(2), 215-21, Language: English, Database: MEDLINE

Nitrogen-containing compounds are one important class of constituents in tobacco because of various pharmacological and biological properties. Three types of tobacco leaves (burley, bright, and oriental) were studied using solid-state (15)N NMR cross polarization with magic-angle spinning, dipolar dephasing and five pi replicated magic angle turning (FIREMAT) experiments. The results show that burley tobacco leaves contain significantly more pyridinic nitrogen than that of bright or oriental tobacco leaves. The principal values of (15)N chemical shift tensors of nitrogen functional groups were obtained from the FIREMAT data. Possible assignments of solid-state (15)N NMR resonances were made using nitrogen chemical shift tensors in some model compounds or isotropic chemical shift values from liquid NMR results. To the best of our knowledge, this is the first solid-state (15)N NMR study of tobacco plant material.

Application of GC-MS/MS for the Analysis of Tobacco Alkaloids in Cigarette Filler and Various Tobacco Species. By Lisko, Joseph G.; Stanfill, Stephen B.; Duncan, Bryce W.; Watson, Clifford H. From Analytical Chemistry (Washington, DC, United States) (2013), 85(6), 3380-3384. Language: English, Database: CAPLUS,



This publication reports the first known use of gas chromatog.-tandem mass spectrometry for the quantitation of five minor tobacco alkaloids (nornicotine, myosmine, anabasine, anatabine, and isonicoteine) in various tobacco samples. A summary of the concns. of these minor alkaloid levels in the filler from 50 popular cigarette brands were found to be 659-986 μg/g nornicotine, 8.64-17.3 μg/g myosmine, 127-185 μg/g anabasine, 927-1390 μg/g anatabine, and 23.4-45.5

μg/g isonicoteine. Levels of minor alkaloids found in ref. cigarettes (1R5F, 2R4F, 3R4F, CM4, and CM6) as well as burley, flue-cured, oriental, reconstituted, and Nicotiana rustica and Nicotiana glauca tobacco types are also reported. Quantitation of the minor tobacco alkaloids is important because the alkaloids have been shown to be precursors of carcinogenic tobacco specific N'-nitrosamines.

Three new flavonoids from the leaves of oriental tobacco and their cytotoxicity. By Chen, Jinxiong; Leng, Hongqiong; Duan, Yuanxing; Zhao, Wei; Yang, Guangyu; Guo, Yadong; Chen, Yongkuan; Hu, Qiufen. From Phytochemistry Letters (2013), 6(1), 144-147. Language: English, Database: CAPLUS,

Three new flavonoids, 6,7-dimethoxy-4'-hydroxy-8-formylflavon (1), 8-formyl-4',6,7-trimethoxyflavon (2), 4',7-dihydroxy-8-formyl-6-methoxyflavon (3), together with fifteen known flavonoids (4-18) were isolated from the leaves of oriental tobacco (a variety of Nicotiana tabacum L). Their structures were detd. by means of HRESIMS, extensive 1D and 2D NMR spectroscopic studies and chem. evidences. The cytotoxicity against five human tumor (NB4, A549, SHSY5Y, PC3, and MCF7) cell lines of compds. 1-3 were also evaluated. The results showed that compds. 1 and 3 showed high cytotoxicity against PC3 and A549 cell lines with IC_{50} values of 2.6 and 1.6 μM, resp.

Oriental Tobacco - Pyrolysis

Investigation of tobacco pyrolysis gases and puff-by-puff resolved cigarette smoke by Single Photon Ionisation (SPI) -Time-of-Flight Mass Spectrometry (TOFMS) By Adam, Thomas; Mitschke, Stefan; Baker, Richard R. From Beitraege zur Tabakforschung International (2009), 23(4), 203-226. Language: English, Database: CAPLUS

The work presented deals with the application of Single Photon Ionization-Time-of-Flight Mass Spectrometry (SPI-TOFMS) for the investigation of tobacco smoke. SPI-TOFMS is a modern anal. technique, which enables the simultaneous anal. of a large no. of org. species in complex gas mixts. in real time. The paper is a summary of a PhD thesis (1) and seven research

articles, which were recently published in various scientific journals (2-8). Consequently, more detailed information on particular aspects can be found in there. The exptl. part covers two different approaches, and therefore, it is divided into two sub-sections. In the first one, the SPI-TOFMS is coupled to a pyrolysis furnace. The objective is to examine the thermal behavior of tobacco under various controlled conditions. In so doing, three tobacco types (Virginia, Oriental, and Burley) were pyrolyzed in two reaction gas compns. (nitrogen and synthetic air) and seven different furnace temps. (400 °C, 500 °C, 600 °C, 700 °C, 800 °C, 900 °C, and 1000 °C). Results can help to unravel the complex formation and decompn. reactions taking place when tobacco is heated. In the second part the SPI-TOFMS is connected to a cigarette smoking machine in order to investigate the behavior of cigarette smoke constituents on a puff-by-puff basis. The work incorporates the comparison of whole smoke and gas phase of cigarette smoke, a puff-resolved quantification of several hazardous smoke constituents, and the overall chem. characterization of the individual smoking puffs. In addn., a crit. consideration of the prevailing smoking procedure is given when applied to single puff anal. A further study examines the influence of five different cigarette lighting devices (gas lighter, elec. lighter, candle, match, and burning zone of another cigarette) on the chem. compn. of the first puff.

Discrimination of three tobacco types (Burley, Virginia and Oriental) by pyrolysis single-photon ionisation-time-of-flight mass spectrometry and advanced statistical methods By Adam T; Ferge T; Mitschke S; Streibel T; Baker R R; Zimmermann R From Analytical and bioanalytical chemistry (2005), 381(2), 487-99, Language: English, Database: MEDLINE

Pyrolysis single-photon ionisation (SPI)-time-of-flight mass spectrometry (TOFMS) and statistical analysis techniques have been applied to differentiate three major tobacco types, Burley, Virginia and Oriental, by means of the gas phase. SPI is known as a soft ionisation technique that allows fast and comprehensive on-line monitoring of a large variety of aliphatic and aromatic substances without fragmentation of the molecule ions. The tobacco samples were pyrolysed at 800 degrees C in a nitrogen atmosphere. The resulting pyrolysis gas contained signals from more than 70 masses between m/z 5 and 170. Mass spectra obtained were analysed by principal component analysis (PCA) and linear discriminant analysis (LDA) to distinguish between different tobacco types. Prior variable reduction of the data set was carried out by calculation of the Fisher ratios. Results achieved give information about chemical composition and characteristics of the smoke derived from each tobacco type and enable conclusions on plant cultivation to be drawn. Based on LDA, a model for tobacco type recognition of unknown samples was established, which was cross-checked by additional measurements of each tobacco type. Furthermore, first results on the recognition of tobacco mixtures based on principal component regression (PCR) are presented.

Changes in the chemical composition of the pyrolysates of various types of tobaccos and selected model carbohydrate compounds in the presence of ammonia releasing agents By Pithawalla, Yezdi B.; Paine, John B.; Rogers Hollins, Sydana; Connell, Chris T.; Fournier, Jay A.

From Abstracts of Papers, 230th ACS National Meeting, Washington, DC, United States, Aug. 28-Sept. 1, 2005 (2005), CARB-089. Language: English, Database: CAPLUS

Following a brief introduction to our Pyrolysis-Gas Chromatog./Mass Spectrometry (Pyro-GC/MS) exptl. setup, the effect of pyrolyzing burley, oriental and bright tobaccos each with a model ammonia releasing agent (ammonium bicarbonate) will be discussed. Comparative GC/MS fingerprinting studies involving pyrolysis of the tobaccos in the absence and presence of ammonium bicarbonate demonstrate that the effect of added ammonia releasing agents on the pyrolysis chem. significantly depends on the type of tobacco under investigation. The effect as defined by the reduced formation of selective oxygenated compds. and the enhanced formation of certain nitrogenous compds. was found to be most dominant for bright tobacco and least dominant for burley tobacco. It will be proposed that either the higher concns. of reducing sugars in bright tobacco or the higher amts. of endogenous nitrogen contg. compds. in burley or both may be responsible for these obsd. effects. To verify one of the above proposed hypotheses, co-pyrolysis of ammonium bicarbonate with selective model carbohydrate compds.; glucose and cellulose was performed. Differences obsd. in the chem. compn. of the pyrolyzate in the presence of ammonium bicarbonate supports the hypothesis that ammonia potentially affects the pyrolysis chem. of the carbohydrate functionality in tobacco.

TG-FTIR analysis of biomass pyrolysis By Bassilakis, R.; Carangelo, R. M.; Wojtowicz, M. A. From Fuel (2001), 80(12), 1765-1786. Language: English, Database: CAPLUS, DOI:10.1016/S0016-2361(01)00061-8

A great need exists for comprehensive biomass-pyrolysis models that could predict yields and evolution patterns of selected volatile products as a function of feedstock characteristics and process conditions. A thermogravimetric analyzer coupled with Fourier transform IR anal. of evolving products (TG-FTIR) can provide useful input to such models in the form of kinetic information obtained under low heating rate conditions. In this work, robust TG-FTIR quantification routines were developed for IR anal. of volatile products relevant to biomass pyrolysis. The anal. was applied to wheat straw, three types of tobacco (Burley, Oriental, and Bright), and three biomass model compds. (xylan, chlorogenic acid, and d-glucose). Product yields were compared with literature data, and species potentially quantifiable by FTIR are reviewed. Product-evolution patterns are reported for all seven biomass samples.

Phenolic compound formation from the low temperature pyrolysis of tobacco By McGrath, Thomas E.; Brown, Anthony P.; Meruva, Naren K.; Chan, W. Geoffrey From Journal of Analytical and Applied Pyrolysis (2009), 84(2), 170-178. Language: English, Database: CAPLUS, DOI:10.1016/j.jaap.2009.01.008

The formation of 10 phenolic compds. (hydroquinone, resorcinol, catechol, phenol, 4-methylcatechol, 3-methylcatechol, guaiacol, o-, m-, and p-cresol) from the pyrolysis of different tobacco types at temps. between 350 and 600 °C was investigated. Hydroquinone,

catechol, guaiacol, 3-methylcatechol, and 4-methylcatechol were formed predominately at temps. ≤350 °C from the primary decompn. of tobacco components. Cresols formed predominately between 350 and 600 °C and evolved from the residual solid (char) that forms at temps. above 350 °C. Phenol and resorcinol were found to form over both temp. ranges, ≤350 °C and between 350 and 600 °C suggesting contributions from both the decompn. of tobacco components and the 350 °C residual solid. The trend in the yields of hydroquinone and catechol obtained from the tobacco types tested; bright (flue cured), burley, and oriental followed bright ~ oriental > burley. All three tobacco samples gave similar yields of phenol and cresols. Water extn. of tobacco was shown to significantly reduce the yields of phenolic compds. The addn. of 5 and 21% oxygen to the pyrolysis setup led to a significant redn. in the yields of hydroquinone and catechol but the yields of phenol and cresols remained relatively unchanged. Quinic acid and quinic acid derivs. present in tobacco are identified as important precursors of hydroquinone, catechol, and phenol.

Oriental Tobacco : Transfer studies

Transfer of organochlorine pesticide residues into cigarette smoke as a function of tobacco blends and filter types By Ceschini, P.; Chauchaix, R. From Beitraege zur Tabakforschung International (1980), 10(2), 134-8. Language: English, Database: CAPLUS

The transfer during smoking of pesticides contained in tobacco into the smoke and the filter of cigarettes was investigated. The overall transfer into the mainstream smoke was 17%, it was independent of the type of the tobacco blend (American, Maryland, Virginia and Oriental). The pesticide retention of the following 4 filters was investigated: cellulose filter, cellulose acetate filter with low and high pressure drop, and a charcoal filter, characterized by nicotine retentions of 38, 27, 48, and 54%, resp. The corresponding pesticide retentions were 40, 21, 39, and 38%, i.e. lower than the nicotine retention in the cellulose acetate, and significantly lower in the charcoal filter. A 3% degrdn. of p,p'-DDT and o,p'-DDT contained in tobacco to p,p'-DDE and o,p'-DDE, resp., was also obsd. The pesticides initially contained in the tobacco part of the cigarette butt decreased during smoking. This appears to be the result of some initial condensation of substances carried through by the smoke stream (as indicated by the presence of pesticide degrdn. products), followed by strong desorption during the very last puffs.

The form of nicotine in tobacco. Thermal transfer of nicotine and nicotine acid salts to nicotine in the gas phase By Seeman J I; Fournier J A; Paine J B 3rd; Waymack B E From Journal of agricultural and food chemistry (1999), 47(12), 5133-45, Language: English, Database: MEDLINE

Thermal transfer to nicotine in the gas phase from neat nicotine, from various nicotine carboxylic acid salts, and from endogenous nicotine in Burley, Bright, and Oriental tobacco samples has been examined by thermogravimetric/differential thermal analysis/mass spectroscopy and evolved gas analysis. Under the conditions used in these studies, the peak transfer

temperatures of these substances to nicotine in the gas phase are nicotine and nicotine acetate, both ca. 110-125 degrees C; nicotine malates, ca. 110-210 degrees C for nicotine to malic acid ratios of 1:0.56 and 1:1 and ca. 160-210 degrees C for a nicotine to malic acid ratio of 1:2; (S)-nicotine bis[(2R,3R)-hydrogen tartrate] dihydrate, ca. 195-210 degrees C; and tobacco samples, a range of ca. 160-220 degrees C. These results suggest that nicotine is mostly protonated in tobacco leaf. In all cases, the temperature of the transfer of nicotine to the gas phase was found to be many hundreds of degrees below the temperatures observed around the coal of a burning cigarette (smolder, ca. 500-775 degrees C; dynamic smoking, 600 to over 950 degrees C). Within the narrow zone of a puffing cigarette that encompasses an intermediate temperature range (125-250 degrees C), kinetic data suggest that these temperatures are not sufficient to volatilize significant amounts of nonprotonated nicotine, assuming any exists at all, during the short puff duration (2 s). It is concluded that nonprotonated nicotine and protonated nicotine (salts of nicotine with natural tobacco carboxylic acids) will transfer nicotine to smoke with comparable yields and efficiencies during the smoking process.

Oriental Tobacco : *in vitro* toxicology

The mouse lymphoma thymidine kinase assay for the assessment and comparison of the mutagenic activity of cigarette mainstream smoke particulate phase By Schramke, H.; Meisgen, T. J.; Tewes, F. J.; Gomm, W.; Roemer, E. From Toxicology (2006), 227(3), 193-210. Language: English, Database: CAPLUS, DOI:10.1016/j.tox.2006.07.019

The mouse lymphoma thymidine kinase assay (MLA) was optimized to quant. det. the in vitro mutagenicity of cigarette mainstream smoke particulate phase. To test whether the MLA is able to discriminate between different cigarette types, specially constructed cigarettes each contg. a single tobacco type - Bright, Burley, or Oriental - were investigated. The mutagenic activity of the Burley cigarette was statistically significantly lower, up to approx. 40%, than that of the Bright and Oriental cigarettes. To det. the impact of 2 different sets of smoking conditions, American-blend cigarettes were smoked under US Federal Trade Commission/International Organization for Standardization conditions and under Massachusetts Department of Public Health (MDPH) conditions. Conventional cigarettes - 8 from the US com. market plus the Ref. Cigarettes 1R4F and 2R4F - and an elec. heated cigarette smoking system (EHCSS) prototype were tested. There were no statistically significant differences between the 2 sets of smoking conditions on a per mg total particulate matter basis, although there was a consistent trend towards slightly lower mutagenic activity under MDPH conditions. The mutagenic activity of the EHCSS prototype was distinctly lower than that of the conventional cigarettes under both sets of smoking conditions. These results show that the MLA can be used to assess and compare the mutagenic activity of cigarette mainstream smoke particulate phase in the comprehensive toxicol. assessment of cigarette smoke.

Oriental Tobacco : smoke chemistry

Investigation of tobacco pyrolysis gases and puff-by-puff resolved cigarette smoke by Single Photon Ionisation (SPI) -Time-of-Flight Mass Spectrometry (TOFMS) By Adam, Thomas; Mitschke, Stefan; Baker, Richard R. From Beitraege zur Tabakforschung International (2009), 23(4), 203-226. Language: English, Database: CAPLUS

The work presented deals with the application of Single Photon Ionization-Time-of-Flight Mass Spectrometry (SPI-TOFMS) for the investigation of tobacco smoke. SPI-TOFMS is a modern anal. technique, which enables the simultaneous anal. of a large no. of org. species in complex gas mixts. in real time. The paper is a summary of a PhD thesis (1) and seven research articles, which were recently published in various scientific journals (2-8). Consequently, more detailed information on particular aspects can be found in there. The exptl. part covers two different approaches, and therefore, it is divided into two sub-sections. In the first one, the SPI-TOFMS is coupled to a pyrolysis furnace. The objective is to examine the thermal behavior of tobacco under various controlled conditions. In so doing, three tobacco types (Virginia, Oriental, and Burley) were pyrolyzed in two reaction gas compns. (nitrogen and synthetic air) and seven different furnace temps. (400 °C, 500 °C, 600 °C, 700 °C, 800 °C, 900 °C, and 1000 °C). Results can help to unravel the complex formation and decompn. reactions taking place when tobacco is heated. In the second part the SPI-TOFMS is connected to a cigarette smoking machine in order to investigate the behavior of cigarette smoke constituents on a puff-by-puff basis. The work incorporates the comparison of whole smoke and gas phase of cigarette smoke, a puff-resolved quantification of several hazardous smoke constituents, and the overall chem. characterization of the individual smoking puffs. In addn., a crit. consideration of the prevailing smoking procedure is given when applied to single puff anal. A further study examines the influence of five different cigarette lighting devices (gas lighter, elec. lighter, candle, match, and burning zone of another cigarette) on the chem. compn. of the first puff.

Levels of tobacco-specific nitrosamines and polycyclic aromatic hydrocarbons in mainstream smoke from different tobacco varieties By Ding, Yan S.; Zhang, Liqin; Jain, Ram B.; Jain, Ntasha; Wang, Richard Y.; Ashley, David L.; Watson, Clifford H. From Cancer Epidemiology, Biomarkers & Prevention (2008), 17(12), 3366-3371. Language: English, Database: CAPLUS, DOI:10.1158/1055-9965.EPI-08-0320

It has been estd. that one in every five cancer deaths worldwide are related to tobacco use. According to the IARC, 10 polycyclic arom. hydrocarbons (PAH) and 8 tobacco-specific nitrosamines (TSNA), as well as at least 45 other compds. or substances found in tobacco smoke, are potential human carcinogens. The levels of these carcinogens in contents of tobacco and smoke emissions vary between different tobacco products. We evaluated mainstream smoke emissions from cigarettes made with different types of tobacco to examine the relation between their deliveries of TSNAs and PAHs and any possible influence from tobacco nitrate content. To investigate the contribution of tobacco content to mainstream cigarette smoke deliveries without confounders such as filter design, filter ventilation, and paper porosity, we used custom-made, research-grade, unfiltered cigarettes that contained bright,

burley, oriental, reconstituted, or mixts. of these tobaccos. Our findings confirm results from other researchers that tobacco type can influence the mainstream smoke delivery of nicotine, TSNAs, and PAHs. However, we found that the effect varies among individual compds. In addn., we obsd. a statistically significant relationship between nitrate content and mainstream smoke 4-(N-nitrosomethylamino)-1-(3-pyridyl)-1-butanone (NNK); nitrate level also influenced the mainstream smoke deliveries of the summed total of the 10 PAHs identified by IARC as potential human carcinogens. The influence of nitrate on mainstream smoke NNK and PAH levels were of different magnitude and direction. Our results tend to indicate an inverse relation exists between NNK and PAH deliveries when considering different tobacco blends.

Puff-by-puff resolved characterisation of cigarette mainstream smoke by single photon ionisation (SPI)-time-of-flight mass spectrometry (TOFMS): Comparison of the 2R4F research cigarette and pure Burley, Virginia, Oriental and Maryland tobacco cigarettes By Adam, Thomas; Mitschke, Stefan; Streibel, Thorsten; Baker, Richard R.; Zimmermann, Ralf. From Analytica Chimica Acta (2006), 572(2), 219-229. Language: English, Database: CAPLUS, DOI:10.1016/j.aca.2006.05.043

Soft single photon ionization (SPI)-time-of-flight mass spectrometry (TOFMS) is applied for the characterization and comparison of puff-by-puff resolved and total yields of cigarette mainstream smoke from single tobacco type cigarettes (Virginia, Oriental, Burley, and Maryland) and the 2R4F University of Kentucky research cigarette. Puff-by-puff characteristics of various smoke components within one cigarette type as well as between different cigarette types can differ tremendously. This is demonstrated by means of a few selected compds. Puff yields vary between 15 and 106 μm for acetaldehyde, 6 and 57 μm for NO, and between 1 and 8 μm for butadiene. Thereby, cigarettes contg. 100% Oriental and Burley tobacco exhibit a very unique behavior for the first and last puff. Different cultivation and processing methods as well as burning characteristics are most likely responsible for this. Since the 2R4F cigarette contains all four tobacco types it combines features of all of them. However, for some smoke constituents, smoking of the 2R4F ref. cigarette results in exceptionally high yields which might not be attributable to the four pure tobacco types, but to other factors. In addn., comparison of the different cigarettes was also carried out by normalizing the yields to puff resolved particulate matter. This procedure minimises effects caused by unequal smoke formation and represents another approach in evaluating the data.

Chemistry of cigarette burning processes By Chen, Peishi From Beitraege zur Tabakforschung International (2004), 21(2), 105-110. Language: English, Database: CAPLUS

A review. Cigarette-burning and the smoke-formation processes and smoke compn. are important topics for understanding cigarette performance. This paper proposes the mol. formulas representing the active components of bright, burley, and Oriental tobaccos and a basic chem. model of the cigarette burning processes. Previous knowledge of the cigarette burning processes and smoke formation helped to establish parameters in deriving the basic

chem. equations. The proposed chem. provides a brief view of the mechanisms of the cigarette burning during puffing and interpuff smoldering, and can be used to interpret and predict the smoke compn. for cigarettes made from bright, burley, and Oriental tobaccos. Based on the proposed chem., the effect of ventilation on smoke component deliveries is discussed and the reaction heat of the puffing process is estd.

TSNA levels in the mainstream smoke of simplified blend prototypes By d'Andres, Sandrine; Boudoux, Roxane; Renaud, Jean-Marc; Zuber, Jacques From Beitraege zur Tabakforschung International (2003), 20(5), 331-340. Language: English, Database: CAPLUS

Different approaches have been reported in the literature to reduce the tobacco-specific nitrosamine (TSNA) levels in mainstream smoke (MSS). The redn. of TSNA in the raw tobacco is an approach that has received much attention in recent years. Different elements det. the level of TSNA in MSS: during combustion, part of the TSNA in the cigarette filler can transfer into smoke while another portion can undergo thermal degrdn. Moreover, it is possible that TSNA can be pyrosynthesized and that concomitant synergetic effects between the blend components can also occur. Depending on their extent, the formation and degrdn. of nitrosamines during the combustion process might have an important impact on TSNA level in the smoke of blended cigarettes and might lead to MSS TSNA deliveries which would not parallel that of the blend components. A study was therefore undertaken to assess the feasibility of predicting the TSNA deliveries of blended products on the basis of the TSNA deliveries of the individual blend components. A highly simplified blend-model was chosen, including laminar Virginia, burley and Oriental tobaccos in fixed proportions. A set of one-, two- and three-component prototypes was prepd. with various combinations of high- and low-TSNA Virginia and burley tobacco. The pre-formed TSNA levels of the different blend components and the MSS delivery of the prototypes were detd. The TSNA deliveries of the blended prototypes were found to be in good agreement with the predictions based on both the MSS TSNA delivery and the pre-formed TSNA content of the individual blend components. This study showed that predicting MSS TSNA levels in the smoke of blended cigarettes could probably be achieved with adequate accuracy from the levels measured in the smoke of the laminar blend components. Strong indications were obtained that such predictions could be made from the pre-formed TSNA content of the raw tobacco. With respect to the redn. of TSNA in MSS, the reported results provided evidence that procuring tobaccos with very low levels of pre-formed TSNA would be an effective strategy to reduce the content of TSNA in MSS.

Chemical variability of mainstream cigarette smoke as a function of aerodynamic particle size By Jenkins, R. W., Jr.; Francis, R. W.; Flachsbart, H.; Stoeber, W. From Journal of Aerosol Science (1979), 10(4), 355-62. Language: English, Database: CAPLUS, DOI:10.1016/0021-8502(79)90029-6

Particles of cigarette mainstream smoke were chem. different, depending on their aerodynamic sizes in the 0.1-0.5 μm diam. range. Anal. of particles >0.5 μm revealed that coagulation probably randomized the chem. compn. In general, distillable compds. were depleted in particles <0.5 μm, whereas pyrolytic products were enriched. In the 0.1-0.2 μm particles, Burley tobacco contributed most to the mainstream smoke total particulate matter, with Oriental tobacco second.

Carbonyl compounds in Bulgarian tobacco smoke By Ivanov, Nikolai; Mokhnachev, I. G.; Kamenshtikova, S. From Comptes Rendus de l'Academie Bulgare des Sciences (1967), 20(4), 313-16. Language: English, Database: CAPLUS

The carbonyl compds. in 9 Bulgarian oriental tobaccos and in the Soviet Ostrolist variety produced in Bulgaria were isolated by chromatog. The volatile compds. gave 19 spots (mostly aliphatic compds.), 11 of which were identified. The nonvolatile fraction gave 17 spots, nonidentified aromatic, oxy, and dioxy compds. The carbonyl compds. identified by paper and gas-liquid chromatog. and quant. detd. photometrically were: MeCHO 0.53-1.18, acetone + propionic aldehyde 0.20-0.42, methyl ethyl ketone 0.15-0.34, isovaleraldehyde 0.20-0.50, valeraldehyde 0.03-0.12; butyraldehyde + isobutyraldehyde 0.09-0.27, furfurol 0.12-0.50; and diacetyl traces to 0.21 mg./g. of tobacco burned. No major differences were found in the quantity of volatile and nonvolatile carbonyl compds. in the tobacco but the organoleptic assessment seemed to improve with an increase in nonvolatile carbonyl compds. and with a decrease in the volatile ones.

Time-resolved analysis of the emission of sidestream smoke (SSS) from cigarettes during smoking by photo ionization/time-of-flight mass spectrometry (PI-TOFMS): towards a better description of environmental tobacco smoke. By Streibel, T.; Mitschke, S.; Adam, T.; Zimmermann, R. From Analytical and Bioanalytical Chemistry (2013), 405(22), 7071-7082. Language: English, Database: CAPLUS

This work detd. the chem. compn. of side-stream smoke (SSS) emissions from cigarettes by laser-based, single-photon ionization time-of-flight mass spectrometry. SSS is generated from various cigarette types (2R4F research cigarette, Burley, Oriental and Virginia single tobacco-type cigarettes) smoked on a single-port smoking machine and collected using a fish-tail chimney device. With this set-up, puff-resolved quantification of several SSS components was performed. Investigations of SSS emission dynamics showed the concn. profiles of various substances can be categorized into several groups, depending on the occurrence of a puff or unaffected by changes in the burning zone during puffing. SSS emissions occurring directly after a puff strongly resembled the compn. of mainstream smoke (MSS). In the smoldering phase, clear differences between MSS and SSS were obsd.

Changed chem. profiles of SSS and MSS might also be important for environmental tobacco smoke which is largely detd. by SSS. Also, the SSS chem. compn. SSS is strongly affected by the tobacco type. Thus, the higher N content of Burley tobacco led to detection of increased N-contg. compd. concns. in SSS.