Time-resolved quantification of volatile aroma compound formation during heat treatment of tobacco leaves: method development and application using PTR-ToF-MS

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Introduction

Heat treatment/toasting of tobacco is part of the cigarette manufacturing process, whereby some flavor compounds are formed through, e.g., Maillard reactions between nitrogenous compounds and carbohydrates or through Maillard reactions of amino acids and reducing sugars. The results of such measurements are a basis for the optimization of the processing conditions towards tobacco flavor compounds during tobacco processing. The results of such measurements are a basis for the optimization of tobacco flavor compounds during tobacco processing.

Experimental

A method for the on-line quantitative determination of aroma compounds in the processing air of a laboratory-scale tobacco dryer was developed, based on Proton-Transfer-Reaction Time-of-Flight Mass-Spectrometry (PTR-ToF-MS). A major advantage of PTR-ToF-MS, compared with PTR-Quadrupole-MS, is the high time resolution (in the range of seconds) that can be achieved while scanning the complete spectrum (i.e., from 0-200 m/z) with a mass resolution (m/Δm) of up to 5,500. A soft ionization takes place by charge transfer from a hydronium ion leading to very limited fragmentation. The development of the quantification method comprised three experimental steps. First, a specific sampling setup was designed that allowed continuous dilution of up to 300-fold. Secondly, the instrument-specific mass discrimination effect was determined by the measurement of known concentrations of a commercially available gas standard. In the third step, the fragmentation patterns for 11 out of 27 aroma substances, for which no literature data on fragmentation was available, were determined using either pure substances or solutions in ethanol. The ion selection for the quantification was made according to the ion abundance and the specificity of the ion for the target compound.

Results

The method allowed the quantification of 27 aroma compounds in the processing air with a precision (RSD, n=5) of 5 to 8 %. The measured levels of aroma compounds ranged from 2 to 30,700 ppb. The limit of quantification (approximated by the 10-fold standard deviation of the blank) was in the single digit ppb range for almost all compound. Except for ammonia, acetic acid and nicotine which were present between 4860 ppb and 630,000 ppb. The evolution of the concentration of the 27 compounds in the processing air could be quantified with a time resolution of 10 seconds.

Conclusion

The developed methodology proved suitable for the assessment of specific processing parameters on the extent and kinetics of the release of aroma compounds during tobacco processing. The results of such measurements are a basis for the optimization of the processing conditions towards tobacco flavor enhancement.