Volatile sulfur compounds (VSCs) contribute to food aroma and flavor in complex ways. For instance, dimethyl sulfide (DMS) and methanethiol (MeSH, cheddar aroma) can be useful additives for flavorists, given appropriate concentrations. Dimethyl disulfide (DMDS) and dimethyl trisulfide (DMTS), however, require stricter control due to their unpleasant smell and lower threshold to human nasal perception.

Both methanethiol and DMS can react under heat and/or the presence of oxygen to create polysulfides such as DMDS and DMTS. The high reactivity of VSCs demands reliable analytical methods which minimize artifacts during sample handling, storage and pre-treatment prior to analysis. The Vocus PTR-TOF is an ideal candidate to analyze volatile sulfur species, since Vocus eliminates time-consuming and artifact-prone sample preparations. Moreover, the large dynamic range and high sensitivity of the Vocus PTR-TOF capture the full naturally occurring concentration range of VSCs, from pL/L (ppt) to µL/L (ppm).

In this example experiment, a sample of egg white in a sealed vial was used as a source of both methanethiol and DMS. The cooked egg sample was left at ambient temperature for five days prior to the measurements. A headspace autosampler delivered the egg headspace periodically over a period of 3 days with an interval of one hour, in order to assure the headspace equilibrium prior to each injection. Measurements of empty vials were used as the baseline series. Tens of nL/L (ppb) methanethiol and DMS were detected immediately after the egg was placed inside the 10 mL headspace vial. Over the course of the experiment, ongoing microbial activities further increased the methanethiol and DMS concentrations by a factor of two to three. DMDS and DMTS increased steadily, reaching concentrations a factor of 100 higher than their initial values. The increase in DMDS and DMTS
is likely due to the fast oxidation of methanethiol and/or DMS. The ability to detect substances of various functional groups, with a large concentration range and fast changing behavior, make Vocus PTR-TOFMS the preferred choice for similar use cases, such as incubator monitoring, process reactor control and other online measurements of ongoing reactions.

Figure 1. Temporally resolved profile of Methanethiol, DMS, DMDS and DMTS during a continuous measurement of 58 hours. Upper panel: Both methanethiol and DMS increase during the first 15 hours due to ongoing microbial production. Bottom panel: The level of DMDS and DMTS grew by more than two orders of magnitude in 20 h. The oxidation of the predominating Methanethiol and DMS is likely the contributing factor. The response factor of xylene was used to estimate concentrations of the organic polysulfides.

References


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