**TGA-PTR-ToF-MS: A Novel System for Comprehensive Analysis of Volatile Products of Thermal Decomposition**

**The aim of the project:** Our goal is to create an analytical tool for investigating the type and amount of volatile organic compounds (VOCs) emitted from a sample as it is steadily heated up in controlled conditions. We want the tool to be very sensitive and to enable the monitoring of dynamic thermal degradation processes in real-time. The emission of VOCs from a sample that is heated to high temperatures and starts to degrade can happen very fast (think for instance of melting plastic that gives off an unpleasant smell). To capture these emissions at that exact moment we cannot simply heat the sample and then quantify what VOCs were generated during that time as a whole. We need to be able to monitor the changes in concentration (or, rather, the mixing ratio) of potentially hundreds of different compounds second-by-second, and to also know at which time point (or at which temperature) the sample undergoes major changes. By combining these two pieces of information, we will be able to obtain a comprehensive and detailed view of what compounds are emitted from a sample at which time point and at which temperature.

**How this will be achieved:** There already exists a method that allows one to heat a sample to an exact temperature in a very controlled manner, at the same time recording how its weight is changing: it is called thermogravimetric analysis (TGA). A tiny amount of material is placed on a very precise scale and heated up to temperatures of over 1000 °C in a stream of gas. The result is a graph showing how the weight of the sample was changing as a function of both time and temperature. To analyse the complex mixture of gases that are being emitted from the sample during that time we will use mass spectrometry. In that technique, the gas molecules are first ionised, and then a sophisticated analyser determines their exact mass, or, to be exact, mass-to-charge ratio, and from the signal intensity, one can also derive their concentration. This is, however, not easy to do directly and in real-time, because the gas stream exiting the TGA, although it contains trace amounts of the compounds we are interested in, is still mostly air, so some 78% nitrogen and 21% oxygen. If we ionise those, there is no way that our detector will register the VOCs at the same time. This is why we will sample the exhaust with a “soft ionisation” technique called proton transfer reaction time-of-flight mass spectrometry (PTR-ToF-MS). In it, only the VOCs are ionised and detected, while the main inorganic constituents of air are not. This makes it possible to monitor the mixing ratio of VOCs in real-time and at 10 ppt concentration level (or approx. 1 drop of water in 2 Olympic-size swimming pools). Thus, we will be able to correlate the changes in the concentration of hundreds of compounds with the weight change of the sample and with the temperature at any particular point in time during the analysis.

**Why This Research Matters:** Understanding VOC emissions during thermal degradation is critical for developing safer materials and mitigating harmful environmental impacts. Existing techniques fall short of capturing the dynamic changes in VOC profiles and critical temperature points where harmful substances are emitted. This project fills a significant gap, enabling scientists to correlate VOC emissions with material behaviour as they are gradually heated to high temperatures. The insights gained could lead to innovative strategies in designing environmentally friendly materials, safer food processing techniques, and improved health regulations regarding exposure to toxic compounds.

**Expected Outcomes:** The project will deliver a novel, sensitive, validated TGA-PTR-ToF-MS system. Subsequently, a series of studies will be conducted to showcase its usefulness in different fields. In **Material Science,** by studying how the composition of polymer blends affects the emission of volatiles during their thermal degradation; in **Food Chemistry,** by investigating the products of Maillard reaction (browning) of micro-dough as it is being baked; and in **Public Health,** by determining the VOCs emissions from tobacco products under controlled conditions, mimicking the real-life smoking habits.