tools including molecular dynamics and nano-structural representations is an exciting area of research currently at its infancy. WG2 aims to provide a framework of collaboration to support such efforts.

On the other hand, new combinations of trace species and pollutants may become relevant and, possibly, give rise to novel possibilities for active control of combustion by-products. These issues are largely dependent on the interaction of hydrocarbon chemistry with trace elements - currently poorly understood - which will be also an active area of research in WG2.

WG3: Chemical and optical advanced diagnostics for Smart Energy Carriers conversion monitoring

WG3 aims to provide a forum for the development and evaluation of diagnostic tools and procedures ranging from elementary reaction rate determination to real time measurements in practical devices. This WG strengthen the exchange of expertise on advanced diagnostic techniques that are a prerequisite to the investigation of SECs and technologies.

Advanced optical diagnostics combined laboratory combustion devices, such as model flame burners with well-defined boundary conditions, are a key element to analyse combustion processes and to study the complex multi-dimensional interaction between fluid mechanics and chemical kinetics. In the last decades, several optical diagnostics, especially laser-based techniques, have been developed and in recent years systematically improved to allow the study of elementary chemical combustion reactions. Optical techniques provide in principle a tool to observe the spectroscopic states of molecules and atoms with high spectral and spatial resolution. Optical techniques combine the advantages of high spatial and temporal resolution and allow sensitive and selective species measurements with little influence to the reacting system. On the other hand, they often cannot provide a comprehensive chemical analysis of the mixture composition of a reacting system. Consequently, optical diagnostics need to be complemented with sampling procedures coupled to powerful analytical techniques, such as gas chromatography (GC) and mass spectrometry.

Because reacting systems are highly sensitive to perturbations by sample extraction or very high-power lasers, it is important to apply several complementary methods, and assess the relative effects of each technique on the measurement. Furthermore, multiple measurements of different parameters are essential because a multitude of interdependent factors are fundamental to the understanding of chemical kinetics and by-product formation in combustion processes. For these reasons different advanced diagnostics, including both non-intrusive optical techniques, like Rayleigh, Laser Induced Fluorescence, Coherent anti-Stokes Raman Spectroscopy, Raman, Laser Doppler Anemometry,

Particle Image Velocimetry, differential mobility based sizing techniques, and absorption spectroscopy (as the ultra-sensitive and quantitative Cavity Ring-Down Spectroscopy technique), as well as intrusive techniques, including GC, photoionization mass spectrometry (PIMS) and photoelectron-photoion coincidence spectroscopy (PEPICO) will be applied, adapted within the WG3 and further enhanced to address the scientific and technological issues of SMARTCATS with the objective of obtaining combined flow field and scalar field measurements (temperature and chemical species concentrations) with different methods for selected reference cases.
For example, PIMS using vacuum-ultraviolet radiation from a synchrotron source has proven to be an exceptionally powerful tool to investigate the chemistry in laminar premixed flat flames, thermal or photolysis reactors, as well as for determining branching ratios of chemical reactions, including isomers identification. In subsequent and ongoing collaborative efforts, other combustion-related experiments are developed to take advantage of synchrotron radiation. In the case of the implementation of PEPICO, the work is for the first time being conducted at European synchrotron facilities.
The work in WG3 aims to improve the knowledge on advanced combustion diagnostics, with a strong focus on technology transfer from fundamental to complex systems, and focuses on:
- advanced sampling and chemical analysis diagnostics,
- laser-based and mass-spectrometric diagnostics in fundamental combustion devices and chemical kinetics experiments,
- elementary reaction rate measurements, including kinetics experiments on elementary reactions at very low collision energies as they allow to test the most accurate quantum chemical calculations,
- chemical markers for combustion performance characterization,
- combustion and emission measurements in complex systems (engines, furnaces, household applications, etc.).
An additional objective of WG3 will be the analysis of global “integral” combustion properties in model flames and in complex systems. These global parameters, like the laminar burning velocity or the ignition delay time, are enormously important chemical kinetics combustion mechanisms validation in different conditions. Therefore, various flame velocity measurement methods (heat flux burner, spherical bomb, counterflow burners) will be integrated in the framework of WG3 and the expertise of the researchers involved will be combined.

WG4: Standard definition for data collection and mining toward a virtual chemistry of Smart Energy Carriers

WG4 aims towards the identification of the main requirements and tools for the development of