WG2 aims to **i**ncrease knowledge on the formation of organic and inorganic combustion by-products in order to improve the sustainability of SECs. The use of unconventional fuels in combustion processes may significant alter quality and quantity of the emitted pollutants with respect to standard fuels. The pollutant tendency of smart energy carriers will be studied by tracing pollutant species typically formed in combustion (carbon monoxide, unburned hydrocarbons (UHC), polycyclic aromatic hydrocarbons (PAH), aldehydes, NOx soot and nano-particles) as well as other classes of pollutants possibly originating from SECs.

The introduction of alternative biofuels, sometimes with significant oxygen content, can result in significant aldehydes emission. Oxygenated pollutants emissions will be more pronounced in the case of advanced technologies operating at low temperatures and premixed conditions. Likewise, trace impurities typically contained in biomass-derived biofuels may either condense into the formation of highly toxic by-products such as chlorinated dioxins and furans, whose chemistry by the way is also poorly understood, or can cause operational problems such as deposit formation.

WG2 will aim towards:

1. increased understanding of pollutants chemistry, through the development of more accurate chemical models and well-targeted fundamental experiments,
2. creation of an inventory of noxious emissions from conventional and advanced combustion devices mainly operating on alternative and sustainable fuels.

The WG2 activity will be focused on the less understood aspects of the pollutant formations that is the formation of soot and nanoparticles. This is an important concern in the combustion of conventional fuels which could be even worsened by the use of alternative fuels. Kinetics of (oxygenated) polycyclic aromatic hydrocarbons, soot and nano-particle formation/destruction in smart carrier conversion as well as their morphological, physical and chemical characterization will be the main issues considered. Although much progress has been made in the last decades, the detailed mechanism of PAH growth and soot inception still remains largely unresolved. The surface chemistry of the soot particles is another topic insufficiently understood. This prevents the development of accurate detailed surface models of particle growth and oxidation as well as the relevant thermochemistry governing the processes of interest. WG2 will aim to consolidate current knowledge and provide directions for further research in those issues.

It is currently ascertained that the soot particle size distribution (PSD) and its chemical composition are more important, at least from environmental and health points of view, than soot particle mass. It is suggested that the combustion of new fuels in novel combustion modes may result in totally different soot typologies. Detailed modelling of soot PSD, chemical composition and morphology based on advanced imaging and analytical experimental techniques and on advanced simulation 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,