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

databases, software and mathematical tools for data collection and handling as well as chemistry optimization using data mining techniques. Definition of "crucial" experiments and simulations, uncertainty and sensitivity analysis in combustion modelling will be key issues to be considered.
WG4 will significantly improve the state of the art promoting:
- definition of specific sets of prerequisites and goals for the establishment of a combustion database that will allow efficient electronic communication of combustion-related data,
- definition of critical raw, experimental and numerical data that needs to be made available for the evaluation and possible future re-evaluation of derived parameters and the format required for their efficient communication., - definition of crucial experiments needed to provide a consistent match between experimental evidence and model validation,
- active discussion and research involving the sensitivity and establishment of error bounds both in experimental data and modelling results. This will also result in a formulation of requirements for model sensitivity and error bounds,
- development of methods, such as those from data mining, to analyse the vast quantities of already existing data in order to provide new insight into the combustion process.
The path from raw data to a kinetic model involves a large number and a wide range of different types of data parameters. A typical detailed chemical kinetic model (such as those produced in WG1) consists of thousands of pieces of kinetic data in the form of rate constants for each reaction (at least three parameters in Arrhenius format) and temperature dependent thermodynamic data for each species. In turn, each rate constant and each set of thermodynamic data are derived from large sets of experimental or theoretical, e.g. quantum mechanical or statistical mechanical data. A single experimentally-derived Arrhenius rate constant is made up of individual measurements condensed down to a single rate constant and often these come from several experiments over different parameter ranges. Theoretical calculations of Arrhenius constants can involve whole potential energy surfaces consisting of hundreds to thousands of individual molecular calculations, which themselves consist of a multitude of configuration and electronic data. It is a goal of this work package to provide the prerequisites for a platform to handle this large quantity of diverse data.
The experiments to validate these models also provide in a wide range of experimental parameters and data. For example, a typical temperature and pressure dependent ignition delay time experiment consists of pressure and species plots over time from which the first and second ignition times are derived. From this raw data, a single parameter is derived. This raw data can be used to evaluate error bounds of the data. The exact value of ignition can be opened to interpretation and the availability of the raw data can be useful for validation. An open discussion within this Working Group will be to analyse how and in what form the communication of all forms of experimental

data, beyond that published in journals, can be improved.

In terms of data collection, storage and usage there are major challenges to overcome. The field of combustion is unique in that the data itself comes from a varying set of scientific communities, such as theoretical and experimental chemists, physicists and engineers, just to name a few. And each one has their own set of requirements and data.

Within the field of computer science there is a multitude of efficient database storage solutions. There are also efforts by groups within the United States to this end. However, the solution is far from final. The challenge lies in the development of standards which satisfy the needs of the multitude of various user groups within combustion. For this reason an active open discussion is needed within the combustion community with the goal of establishing specific guidelines for the construction of an efficient database that satisfies the users within the combustion community. The members of this COST Action represent a cross section of these researchers and thus an excellent basis for a complete and thorough discussion.

The main challenge of this WG is to provide a forum for all experts in the combustion community to formulate a common set of requirements for a universal combustion database not only capable of efficiently store the vast amount of raw data generated by experiments and modelling but also, more importantly, efficiently accessible for future use and maintenance.

WG5: Integration of fundamental knowledge towards technology application for Smart Energy Carriers exploitation.

The aim of WG5 is to apply/integrate the knowledge tools developed in WG1-WG4 by means of a mutual exchange between academic and industries. This will provide optimized ready to use tools and techniques for an effective use of SECs on large scale.

The research activities of the WG will be driven by the identification of validation test cases, identified in collaboration with the industrial partners to provide scale-bridging information from the laboratory units to the real applications. Such test cases will need to share important similarities with the intended applications (internal combustion engines, gas turbines, furnaces), without the complex interactions characterizing the industrial systems.

Integration of detailed kinetic mechanisms in large scale numerical simulations.

Detailed kinetic models are crucial to properly understand fuel and combustion properties such as ignition, heat release and pollutant formation. Comprehensive chemical schemes for the SECs and the related pollutant formation pathways will be available from both WG1 and WG2. An objective of WG5 will be to develop methodological approaches and tools for the integration of detailed