DESCRIPTION DU PROJET ET IMPACT ATTENDU/ *PROJECT DESCRIPTION AND EXPECTED IMPACT*

1.1 PRESENTATION SCIENTIFIQUE DU PROJET POUR LA PROCHAINE PERIODE DE FINANCEMENT ET IMPACT ATTENDU / *SCIENTIFIC SCOPE AND CONTENTS OF THE PROJECT FOR THE NEXT FINANCING PERIOD, EXPECTED IMPACT*

The current CAPRYSSES Labex is structured in **3 work packages**:

(A) Internal combustion engines, gas turbines and gasification systems
(B) Aerospace propulsion systems
(C) Industrial risks caused by chemical explosions.

The proposed **CAPRYSSES-2** is an extension of CAPRYSSES keeping the **same WP** and including several **new actions**, as described in the following paragraphs. **Novel subtopics** include principally: **plasma assisted combustion, plasma assisted ignition, biochar, debris (re-)entry and plasma ablation**; the GREMI lab (UMR CNRS-UO) will join the Labex.

Laboratory	Permanent staff involved	Participation to WP
ICARE	21 (4.85 ETPT)	A, B, C
PRISME	31 (6.3 ETPT)	A, B, C
GREMI	9 (1 ETPT)	A, B

WP-A: ICARE and PRISME laboratories have expertise and the worldwide recognition in the analysis of physico-chemical phenomena of combustion and their industrial applications. Kinetics mechanisms and physical models will be improved especially for real applications such as burners for power plants, internal combustion engines, gas turbines… These investigations will be performed using a large range of high quality experimental facilities: JSR, shock tube, RCM, micro-channels, high pressure laminar and turbulent burners of gaseous and two-phase combustion, high pressure and high temperature spherical combustion chambers for premixed flame and spray analysis coupled with many experimental techniques such as GC, CRDS, mass spectrometry, optical diagnostics or others. CAPRYSSES expertise in high-temperature reaction kinetics could be extended to other systems than combustion, e.g. reactions in volcanoes plumes in interaction with Labex VOLTAIRE In addition, the expertise of CAPRYSSES partners in combustion studies will be extended to other chemical conversion processes such as hydrothermal processes in order to generate useful energetic materials such as bio/hydrochars from the conversion of wet organic waste materials. Hydrochars are alternative solid fuels but also have strong potential for carbon sequestration and soil remediation. These last two topics could be explored with partners of labex VOLTAIRE, Linyi Univ., and Shandong Univ. through the project 'BIO-CHAR for the optimization of biochar-based microbial biofertilizer and its effect on soil remediation and greenhouse gas mitigation' submitted to the 2018 PRC CNRS–NSFC.

● From capturing CO_2 emissions to zero emission systems: Oxy-fuel combustion is one of the leading technologies considered for capturing CO_2 from large-scale facilities (thermal power plants, steel, cement or glass industries). This involves burning the fuel with nearly pure oxygen instead of air or with oxygen-enriched air. The CO_2-Energicapt program, funded by the ANR (2011-2013), enabled the demonstration on an industrial scale of the effectiveness of CO_2 capture by the membrane route. This demonstration was made possible thanks to a close collaboration between the academic world (ICARE, LRGP) and the industrial world (LLT Leroux and Lotz technologies, Polymem, CPCU). Hydrogen may be seen as a possible candidate to store electricity overproduction from renewables. Ammonia and metallic microparticles may be considered as new zero-CO_2 emissions energy carrier options, especially for long-term energy storage. They have the potential to create a major breakthrough in addressing climate change and primary energy depletion. The high energy density inherent to reactive metals, which motivates their use as additives to propellants and energetic materials, or as anodes within batteries, also inspires their use as recyclable solar fuels. Several projects have been submitted in this area and research is in progress through grants from PSA and through CAPRYSSES-Vrije Univ. Brussel (VUB) collaboration (PhD Thesis of Lhuillier on ammonia combustion, 2017–)

- Biofuels/efuels/sfuels and waste fuels: The development of a sustainable energy vector is a major step for a global warming mitigation. Liquid and gaseous biofuels could play a crucial role in energy storage and CO_2 emissions issues. Valorization of waste and use of green electricity are attractive means to produce biofuels. Biomass/waste gasification in supercritical water or plasma-assisted is a promising pathway. Characterization of the combustion properties of potentially produced fuels must be performed under thermodynamic conditions close to those encountered in real applications. Ongoing projects (PhD of Missaoui on HTC) in this area will continue with CAPRYSSES support.
- Optimization and control of power units: Improving power systems and industrial burners towards clean combustion, i.e. ultra-low pollutant emission, is a great challenge. Chemical improvers (O_3, NO, HCCO, Cetane improver, octane improver, metallic particles…) has shown very promising effects on the combustion process in internal combustion engines. Their effects in Spark-Ignition, Gasoline Compression Ignition, Spark Assisted Compression Ignition or Low Temperature Combustion engines need more efforts to propose new concepts. Plasma-assisted ignition will be performed, extending the current ANR CICCO project (PRISME and GREMI). Due to geopolitical issues and the integration of renewable resources, the French natural gas network is expecting great variations of gas composition in a close future. These trends may lead to adverse impacts on the combustion performances and pollutant emissions of power units (powertrains, gas turbines, APU). Real time adaptation of power units to gas quality will be essential. This requires prior knowledge of the combustion properties of potential mixtures. For heavy-duty engines (trucks, APU and industries), new Engine Control Unit (ECU) strategies must be developed; systems able of monitoring and regulating the combustion status in real time are needed to maintain optimized performances despite gas composition variations.
- Plasma assisted combustion to stabilize flames and control pollutant emissions (ICARE/GREMI): The originality of this approach lies in the coupling between the electricity, on the one hand, by the formation of a gliding arc, pulsed arc or multi-jet glide plasma, and, on the other hand, the combustion of the fuel. This plasma-assisted combustion is likely to stabilize the flame and control pollutant emissions. An industrial producer of cooking appliances (Brandt Cooking) is interested in this project. We will study the effect of the gliding arc on the flame behavior as a function of the various plasma parameters (frequency, voltage, etc.) and flame parameters (flow, richness, etc.). The shape, size bond and stability of flames will be analyzed. Chemiluminescence experiments coupled with spectroscopy will be performed in the presence of plasma and flame. Combustion gas analyzes will be performed without and with plasma. The effect of the gliding arc on polluting emissions (NOx, CO) and CO2 will be studied according to the different plasma and flame parameters.
- High-temperature reaction kinetics beside combustion: Atmospheric effects of high-temperature

emissions from volcanoes, fires, flaring… (ICARE, Labex VOLTAIRE). Emissions, either natural (volcanoes, vegetation, fires) or from human activities (combustion engines, flaring…) release highly reactive chemical compounds and aerosols to the atmosphere through high-temperature processes. The expertise of CAPRYSSES in high to low temperature kinetic modeling could help understanding these processes whereas strengthening its scientific leadership. This project will help quantify the role of these emissions of a complex cocktail of gases and aerosols to the atmosphere, first at high-temperature and then in the low-temperature plumes. When the plumes disperse, the rapid gas-phase and heterogeneous photochemistry affects atmospheric ozone, pollutants and aerosol burdens, therefore impacting air quality and climate regionally but also far from the source through wind advection. Building on a new synergy between teams in Orleans, this project brings advances through the use of reactive plume modeling methods, recently developed in LPC2E (member of the Labex VOLTAIRE and Equipex PLANEX), to derive simultaneously the gas composition and aerosol properties from the source emissions and throughout the atmosphere. ICARE's experience with high-temperature chemical processes will allow initializing the model with suitable kinetic and thermochemical parameters and identifying the most relevant key compounds and reactions to be investigated. High- to low temperature detailed kinetic mechanisms will be developed in order to predict the evolution of sulphur, halogens, or NOx in the plumes. PRISME will contribute to improving the plume modeling by determining the influence of the microscale environment (orography) and the buoyancy effects of the plume during the first steps of the atmospheric dispersion process.

WP-B: From low speed flows featuring ground vehicles to high speed flows characterizing space applications, the performances of aerospace bodies are intimately connected to the physical mechanisms at play near the fluid-solid boundaries. The development of the boundary layer over slip or non-slip conditions at the wall, its eventual interaction with shock waves, the laminar-turbulent transition or the onset of flow separation are typical examples of the interactions between the wall and the flow. These phenomena are the origin of harmful effects having important impacts such as energy losses, production of disturbances, system threatening or health hazards. Basically, these detrimental effects are strongly dependent on drag induced by friction, pressure gradient and/or shock waves. Over the past decades, flow control has appeared as an attractive way to mitigate these detrimental effects. To this end, a wide range of actuators and control strategies have been developed from passive to active flow control. Although very good results have been reported at the laboratory scale, the success of extrapolation to real life is generally limited. This means that a in depth understanding is missing and accordingly fundamental investigations are of primary interest to bring new insights about the physical mechanisms at play. The main objective of the WP-B-Aerospace propulsion is to tackle this issue by taking benefit of the complementary skills of the two laboratories involved within the labex CAPRYSSES, which have a recognized expertise in fluid mechanics and flow control from low to high speed flows. The project of this WP will target the investigation of the wake of prototype bluff bodies featuring aerospace applications with a specific focus on the atmospheric re-entry (being accidental or not) of aerospace systems. The prediction and eventually the control of the falling trajectory are fundamental issues connected to the wake physics. For example, during deorbiting, space crafts and satellites experience strong forces and thermal effects leading to their destruction, which results in the generation a large number of fragments. The problem of the motion of the cloud of debris become very complex due to the interplay between shock waves and wakes, making the estimation of their trajectories very difficult and inaccurate. At the same time, re-entry of aerospace vehicles is featured by different flight phases (from rarefied conditions at high altitudes to subsonic regime at low altitudes) requiring that the control of the falling trajectory has to be adaptive. The ultimate goal of this WP is to address these issues. To achieve this goal, the action plan of this WP has to be designed to gain a deep understanding of the physical mechanisms driving the wake development of bluff bodies over a wide range of operating conditions. To this end, we will take the benefit of a unique experimental platform bringing together facilities capable of generating flows from subsonic (PRISME) to hypersonic regimes (ICARE). The new insights emerging from WP-B will have two main conclusions: (i) improve the modeling of wake flows and (ii) design new control strategies potentially effective over the entire flight. Combining the complementary tools together with the skills developed by the partners of CAPRYSSES will give an original way to go beyond the current state of the art. Thanks to the CAPRYSSES leverage and the advices from the HCERES and the International Advisory Committee (May 2018, http://caprysses.fr/actu.html), numerical modeling will be reinforced by recruiting a new assistant professor at Polytech'Orléans and PRISME (ESA group, 2018). The methodology that will be deployed to achieve these objectives is briefly described in the following section.

- Flow physics underlying bluff-body wakes: Wake flows are characterized by complex physical interactions making their modeling and understanding challenging issues which are usually addressed through time-consuming trial and error procedures. Fundamental investigations are then essential to bring new insights on the physical mechanisms underlying the development of wake flows at both low and high speeds. One of the main issues which arise is the universality of scaling laws from subsonic to supersonic regimes. As a starting point, the recent progress achieved on the key role of entrainment in separating/reattaching flows (Stella et al., 2017) will offer an attractive way to unify the physics underlying these regimes. To this end, the investigation of entrainment will be extended to wake flows over a wide range of operating conditions in the experimental facilities of both PRISME (subsonic) and ICARE (hypersonic). Sophisticated optical diagnostics will be deployed to estimate the rate of entrainment and its dependency with respect to control parameters such as the Reynolds number, the Mach number or the body aspect ratio.
- Flow control of bluff-body wakes: Over the last past decades, flow control has attracted increasing attention to mitigate the defects of aerospace systems (Debien et al, 2016; Coumar & Lago, 2017). It turns out that in depth knowledge of the scaling parameters driving wake flows is a cornerstone to design efficient control systems and to ensure scalability from laboratory to full-scale applications. Indeed, even for black box approaches, the effectiveness of a control loop will depend on how well design parameters (e.g. sensor/actuator choice and location) match flow parameters (e.g. natural frequency, sensitive regions). The new insights arising from Task 1 will be at the basis of the design of control strategies effective over a wide range of parameters. This original approach will be assessed by targeting the vectoring of a re-entry capsule with the aim to stabilize its falling path. Deploying the control strategy in both subsonic (PRISME) and supersonic/hypersonic (ICARE) facilities will enable to simulate the different flight phases of the capsule or other re-entry bodies. To achieve this goal, different actuations (e.g. fluidic, plasma, mechanical) will be combined depending on their relative efficiency in comparison to the flight phases. The effect of slip conditions at the wall to improve design and aerodynamic performances will be further investigated (GREMI PRISME).

The study of wake interaction phenomena is one of the problems that must be taken into account when dealing with the atmospheric re-entry of space debris such as satellites or spacecraft boosters, because it has a strong influence on their trajectory and impact location. The knowledge that will be gained from this collaboration is of great interest to this new research topic where the expertise of CAPRYSSES in atmospheric entry investigations together with unique CAPRYSSES ground test facilities is a major asset. Under certain conditions, the fall of space debris passing through the dense atmospheric phase, where high temperatures are reached, ends with its complete destruction due to fragmentation and ablation. During ablation phenomena, aerothermodynamics of space debris will change modifying the wake structure. In addition to aerodynamic aspects, this process will produce dust and particles that will contribute in part to the accumulation of aerosol particles present from the ground to the upper atmosphere (~100 km). The origin is mainly due to dust coming from comets, and from the meteoritic disintegration but a quantity becoming each year more important provides from artificial debris. From an environmental point of view, dust play a major role in the radiative balance of the Earth's atmosphere and thus in climate, and in chemical processes such as those destroying the stratospheric ozone layer. The effects of the aerosols on the atmospheric chemistry and on the climate system depend on their physical properties: size distributions from tens manometers to hundreds of micrometers, morphology and composition. Among the facilities platform of the Labex Caprysses, the PHEDRA wind tunnel is used to experimentally simulate high specific enthalpy (up to 55 MJ.kg-1), low pressure (1 Pa to 100 Pa, simulated altitude: 50 km – 80 km) and supersonic (Mach number > 4) flight conditions in the upper layer of the atmosphere. In view to study how ablation space debris can affect the composition of atmospheric dust, the plasma wind tunnel Phedra will be used to reproduce atmospheric entries simulating space debris in terms of geometries of interest and materials. Molecular Dynamics simulations will be carried out at GREMI for describing elementary processes of erosion under these conditions. They will provide the erosion rates, molecules and radicals formation in the vicinity of the debris surface. These will be compared with the experimental results for a deeper understanding of the erosion processes and will enable to predict debris evolution and dust composition in the atmosphere. This topic is also linked to research topics of the Labex VOLTAIRE and will benefit to both groups. Indeed the LPC2E laboratory, member the labex VOLAIRE , performs in situ detection of aerosol particles with a balloon-borne light aerosols counter' LOAC' that they have developed and used to monitor the stratospheric aerosol content in which natural and artificial debris particles can coexist. Their research field focuses on 'natural debris' such comets and meteorites particles, nevertheless, their expertise and knowledge in aerosol particles can be of great interest for the labex Caprysses regarding investigations of atmospheric entries of artificial debris. Moreover, this scientific synergy between both Labex will be increased through the use of valuable facilities from labex Voltaire that can provide the morphology and composition of the samples obtained in the ICARE laboratory facility from 'debris ablation'.

WP-C: Explosion hazards in industry are not only responsible for tremendous financial losses but more importantly for severe injuries and fatalities. These tragic events can lead to unforeseeable consequences both at political and social level. Understanding chemical explosions is one of the major issues that face the industry and the regulation agencies as well as the lawmakers drafting national/international regulations. Investigating the ability of a given combustible system to ignite and induce a strong energy release is the subject of a continuous effort of both ICARE and PRISME laboratories. Whether the studies are aimed at investigating the risk of Hydrogen explosions in nuclear power plants or due to a reservoir leak in a chemical plant, dedicated experiments are used to investigate: (i) flammability limits, (ii) combustion regimes from laminar to turbulent flames and (iii) fast flames and detonation. Mitigation of explosions is also being the focus of several studies at ICARE. These studies are performed within national programs (PIA-RSNR 'MITHYGENE', ANR-IRSIS, CNES° and international collaborations (SAMHYCO-NET, ETSON, Nagaoka Univ., HYMERES).

● Flammability Limits: Flammability limits constitute one of the combustion parameters that are fundamental to the assessment of the explosion risk. In the framework of nuclear power plants safety, flammability limits of hydrogen based mixtures have been already studied as well as for gas turbine applications using either laser or spark ignited mixtures. The effect of several methods of mitigation, such as diluents, fire suppressants and water spray, will be further investigated, within international programs (SAMHYCO-NET, ETSON group, HYMERES project which is in preparation).

● Explosion Dynamics: Hydrogen is foreseen as energy carrier for the future leading to the concept of a "hydrogen society". Indeed, the absence of carbon atoms makes it suitable to alleviate the greenhouse gas emissions. However, its combustion properties such as a very wide flammability domain and very low ignition energy are responsible for the explosion hazards when a leak occurs in a confined environment. Following a local ignition, the combustible mixture would give birth initially to a slow flame that will rapidly accelerate due to turbulence generated by the confinement. This strong flame acceleration induces high loads that can destroy an industrial building. The research concerning these phenomena will be pursued thanks to the unique facilities such as large spherical bombs (BS-III), flame acceleration vessels (ENACCEF I & II) which are used worldwide for benchmark exercises within the OECD framework (SAMHYCO-NET, ETSON group, HYMERES project). These studies will target H2/CO/CH4/O2/Air mixtures either containing metallic particles (ITER-safety analysis) or water droplets (Pressurized Water Reactor safety analysis). Hybrid mixture explosion (liquid sprays, dust and solid aerosols) characteristics will also be investigated both by PRISME and ICARE. Finally, Detonation studies focused on the dynamic parameters (detonation cell size, speed, and overpressure) will also be pursued emphasizing the chemical kinetics mechanisms involved within the detonation wave. With LGPC laboratory in Lyon, the investigation of the effect of metallic foams on the suppression of a detonation wave in hydrocarbon/air mixtures is being performed (ANR – IRSIS).

● Blast effects induced by detonation: In contrast to the expensive computational time and capacity required by CFD simulations, analytical methods for evaluating the characteristic parameters of the blast wave after an explosion are useful, despite their limitations. Their rapid implementation is useful for a preliminary, on-site study in an emergency situation. However, their improvement is necessary by adding more realistic and physical models. An original method will be developed based on the small-scale experiments allowing detailed phenomenological analysis of combustion and shock wave propagation by including all characteristics parameters of the pressure field. The analysis will constitute the basis for developing predictive numerical methods for large scale systems.

2 JUSTIFICATION DES MOYENS DEMANDES / FUNDING JUSTIFICATION

2.1 JUSTIFICATION DES DEPENSES/EXPENSES JUSTIFICATION

The available funding (8% management fees deducted) of 1,320,132 € will be used for salaries of contract people (1,150,000€) and consumables and missions (170,132€). A total of 450 person.months will be supported by the Labex: (i) Master students internship(salary and a grant equal to 25% of salary for research activities, consumables; 150 p.m.), (ii) Ph.D. students (salary and a grant equal to 25% of salary for research activities, including travel and participation to conferences, consumables; 144 p.m.), (iii) postdocs (salary; 120 p.m.), (iv) salaries of research engineers working on funded projects of WP-

A, B, C. (36 p.m. shared between the Labex laboratories, as in current CAPRYSSES). A total of 137,130 € will be spent for research support (corresponding to 25% of salaries of Master and Ph.D. students). A total of 20,000 € will be spent to host invited researchers (cost 3500–4000€/month per person). A total of 33,000 € will be spent to support training and education activities. A total of 20,000 € will be spent for exploitation of results, database management.

2.2 PLAN DE FINANCEMENT/ FUNDING PLAN

Co-funding of Ph.D. grants by industry and other institutions will be promoted, as in the current Labex (with DGA, VEOLIA, ENGIE, Vrijn Univ. of Brussels, Région Centre VL, Région Bourgogne, Labex EMC3 'Energy Materials and Clean Combustion Center'). Funding from the institutions (permanent staff salaries), PhD grants from Région Centre and Government, and research contracts signed for the duration of CAPRYSSES-2 are given in the following Table:

Institution / Funding	Permanent staff (k€)	PhD grant (number)	Total budget (k€)
UO and INSA-VL	5,700	–	5,700
CNRS	1,200	–	1,200
Région Centre	–	10	1,000
Government(MESR)	–	10	1,000
FEDER/CPER	–	–	3,950
ERC Starting grant	–	–	1,360
Research contracts	–	–	5,057
TOTAL	6,900	20	**19,267**