Labex CAPRYSSES Review Committee

Orléans, May 28, 2018

Introduction

The review of the Labex CAPRYSSES was undertaken during one day. It included a general presentation of the Labex including an overview of the research and education activities, four individual presentations on research results and future plans and perspectives of the individual work packages, and three presentations introducing different Inter-Labex activities. In addition, a report was provided for the review committee with details on these different activities.

This report provides general comments on the center activities and on the different research areas.

General Comments:

Overall - The review committee is very impressed with the level of accomplishments of the Labex CAPRYSSES in term research and education. The center is a lighthouse project in the area of energy transformation, safety, and other topics mostly related to energy and energy transformations. This is evidenced by the large number of scientific publications including more than 50 peer-reviewed publications and an impressive number of awards for the PIs including ERC advanced and starting grants and a Gold Medal of the International Combustion Institute. The PIs are a world-class group of scientists in chemical kinetics of combustion, particularly on the behaviour of high pressure combustion, as well as on high speed aerodynamics. Particularly notable are the combined facilities (shock tube, RCM, PFR, laminar flame vessel), the expertise in chemical kinetics, and the unique capabilities in accessing a range of Mach numbers of relevance to the aerospace industry.

Caprysses maintains collaborations to the most prominent research groups in the area of combustion research and to many companies. This attracts substantial external funding. The report quotes 10 million Euros from other government funds, EU, and industry, which allows for broadening the research areas and to transition the fundamental research funded by the Labex to an applied and industrial level. The mix of work packages in Caprysses is powerful: all are related to energy conversion in fluid-based systems and all address fundamental topics important for our society.

Despite the fact that there is a strong emphasis on experimental work, most of the funds are spent for research staff. Funds for experimental equipment and operation seem to come from other sources. This is commendable and increases the research and educational impact of the center.

In addition to the research activities, the Labex Caprysses supports a large number of educational activities including workshops, conferences, training, summer schools, and more than 50 research seminars.

Specific suggestions:

- It would be helpful to have some keywords to describe the focus of the future proposal: while this is reasonably clear in relation to Caprysses, it is not clear how Caprysses and Voltaire programmes are related to one another.
- In discussion, it appeared that at least part of the motivation for applications to Labex is sustaining existing research programmes. There seems to be a political imperative of focus on consolidation of academic groups, but this is not the same thing as their motivation. In any case, these programmes evolve – so it would be helpful to have sense of overall strategy.
- It appears that its definition is included in the Labex proposal and that this is reviewed. The direction of the research is presumably provided by the senior academics only, assuming it is, in part, driven by industry needs. Some clarification here would be helpful.
- The Steering Committee does not have industry or end-user representatives.
- The excellent research is quite near end-user, with several publications appearing at industry meetings (eg SAE). However, some clarification of the interaction with industry would be helpful, for example, descriptions of mechanism through which these research outputs are communicated directly to industry, especially considering that France has a several large-volume car manufacturers.
- Large grants such as Caprysses often generate important "so what?" questions – what are the outputs of Caprysses which would not be available without it? At the meeting, the answer to this question was very good – namely that often industry wants very specific outcomes, which may not reach the public domain so not for general benefit. Even so, the comments above remain: the financial leverage by Caprysses from industry could be made clearer.
- It would be interesting to have a better sense of where the excellent research ideas come from. Is this from single individuals or groups? The presentation of research projects from is very interesting.
- The idea of a 'virtuous circle' of research finding is not without merit: grant outputs connect with end users (industry) who then agree to co-fund further projects to help develop ideas.
- The IP of research projects does not seem to be identified. Are there exploitation mechanisms? Descriptions of routes for patenting, product licensing and the setting up of new spin out companies for exploitation would be helpful.
- We can see that there is a creative framework underpinning the research, but there appears to be an overriding motive of aggregation – 'big is beautiful'. But there may be a risk of weakening the project definition – at some point, the criteria for excellence have to be clearly articulated at some research directions sacrificed should they be considered as to weak for inclusion.
- While this is likely the case for all work packages, WP-C impressively demonstrated research on all aspects of the industrial safety from very fundamental all the way to the applications. This is possible through funding from other government or industry sources that allow to make the connection to the more applied research. If this is the case for the other work packages, it should be clearly pointed out in the follow-on proposal.
- Some regions of parameter space are better investigated by simulation (eg low Reynolds number) so these types of studies complemented experimental ones quite

well. The hypersonic flow subject to plasma forcing is a case in point. The complementary approach of simulation is not always clear.

- It would be nice to see how Caprysses is integrated with computational work, and equivalent industrial work. Note that numerical activities could be developed further within collaborations such as the one already existing with IMFT and CERFACS.
- For the actual review of the international advisory committee, overview talks would be more helpful than just single topics in more depth.

WP-A Part I: Internal combustion engines, gas turbines and gasification systems

The project has focused on the use of oxygen enrichment, hydrogen enrichment and the use of biofuels.

The oxygen enrichment project has been particularly original with a focus on plasma generation of ozone (O_3), and the effects of reactive species nitric oxide (NO), (NO_2), nitrous oxide (N_2O) and ozone (O_3) on the rate of combustion and emissions in engines operating under homogeneous charge compression ignition (HCCI) or low temperature combustion (LTC). Each of these species accelerates the reactions of hydrocarbon fuel with air. These systematic additions of reactive species reveal details of the chemical kinetics of auto-ignition ignition inside of combustion chambers.

The program is helpfully connected to systematic chemical kinetic measurements in well controlled situations (e.g. plug flow reactors, shock tubes), and for a variety of fuels, thus allowing the generation of detailed chemical kinetic models, which can then be used in the prediction of combustion in engines.

Importantly, the programme is well connected and funded jointly with engine OEMs, creating a pathway for the use of the technique, and developing an engine control strategy for both smooth operation and low emissions. The prospects for the use of an ozonator are practically possible, as the engine consumption is modest, so the eventual decision of whether to exploit the possibilities is limited by the economics of application.

The project on biogas hydrogen addition also focused on the chemical kinetic aspects of combustion of oxygenated and bio-derived fuels, leveraging the good experience of the group in this area.

The biofuels interlap work on hydrothermal carbonisation was not entirely clearly connected, and a clear lifecycle analysis on the overall proposed approach was perhaps not very convincing.

Overall the lab clearly has continued to produced world-leading research in the area of chemical kinetics applied to fuels combustion as applied to engines and related systems, and the database and models emerging from these related experiments have the most long term value to the scientific community.

WP-A Part II: Turbulent Gaseous Combustion

The presentation focused on a very specific and very interesting subject; the development and the investigation of a premixed flame vortex interaction rig to characterise the

influence of fluctuating stretch rates, split into tangential strain and curvature contributions, on the flame consumption and displacement speeds. Diagnostics combine Mie scattering and PIV and experimental data are successfully compared with a two Markstein number theory for methane and propane fuels. Very fruitful collaborations have been set with T. Poinsot's team in Toulouse (isolation of strain and curvature effects) and A. Steinberg in University of Toronto (unique results of ignition ahead of the main flame front when using hydrogen as fuel). Further works are planned to investigate the inner flame structure combining laser Rayleigh scattering, CH* and OH* chemiluminescence. This experiment will also be a relevant target for direct numerical simulations and should be used for modelling.
The new facility could also be useful for other researches, such as the impact of stretch rates on soot in non-premixed flame (if the facility can be adapted to run in non-premixed mode).

We presume the presentation deals with only a small part of the program on turbulent flames. However, no other work is described in this area in the report distributed to the committee. If that is the case, this research area seems quite subcritical and rather isolated inside the Labex program. It should probably be strengthened and/or more connected to other tasks.

WP-B: Aerospace propulsion systems

The group is clearly effective at researching fundamental science that is driven by societal need. It is one of the leading groups on vehicle wakes in France and internationally. The work is adventurous and challenging, with high-calibre outputs.

A key strength is the deliberate cross-fertilization of sub-groups working in different topics, in this case high- and low-speed flows.

- Some aspects of these flows are very different: one in which the density changes faster than the velocity is clearly different to one in which the opposite is so. To try and unite modelling concepts for both low- and high-speed applications should be treated with caution.
- However, near the surface, a shock-wave boundary layer interaction can promote separation which can have a low-frequency oscillation associated with an absolute instability. This is also the case for low-speed flow over a backward-facing step: a connectively unstable mixing layer gives rise to a Kelvin-Helmholtz instability. Below this, there is a recirculation region, which acts as a pocket of global instability casing a lower frequency global oscillation, or 'flapping'. This commonality could be focused on rather more.
- Other common areas of interest exist: tracking the TNTI entrainment interface is not unlike that of a flame front or a shock wave.
- Two queries relating to plasma discharge control of boundary layers at M = 2 – 20:
    - It's the change in voltage that generates the plasmas, and hence the body force. What is the *change* in Knudsen number due to the forcing? Is it sufficient to change the importance of (the degree of) rarefaction?

    - The angle of the leading-edge shock changes due to the effect of the forcing and this could be seen as just a result of additional viscous blockage. But it could be more than that since the forcing occurs below the sonic line. Hence information (change in boundary layer details below the sonic line) can propagate upstream to the leading edge.
- Low-speed separation control – geometry appears to be determined by another project. So to, the forcing jet geometry. This is perhaps not optimal – a 'thought' experiment to prove or disprove a particular idea might require a different configuration.
- Questions of the energy budget were not addressed. The report and presentation clearly identify the need for modelling for flow control. Actuation is expensive in flow control, but an obvious way of minimizing the duty cycle of a system is to use feedback control to optimize the system effectiveness. Real-time control of wind tunnel experiments is now feasible, even with MIMO systems.
- This programme of research could be extended to include real-time control – it provides an opportunity for model-based control, and therefore an examination of the fundamental processes at work.

WP-C: Industrial risks caused by chemical explosions

The work package on industrial safety touches underpins the fundamental understanding of the science of the development of flammability limits and detonation, with a focus on hydrogen mixtures found in nuclear power plant accidents, but also on metal propellants.

A number of well-instrumented and rather unique facilities have been used to investigate a variety of phenomena, including:

- Flame propagation: both laminar and turbulent flame propagation in hydrogen mixtures over a range of conditions, for low and high pressure, laminar and turbulent
- Developing detonation: intrusive (cell size measurement) non-intrusive (pressure, concentrations) measurements to determine the speed of propagation with a range of chemical compositions of hydrogen and nitrogen dioxide mixtures.
- Practical studies of developing detonations in mixtures propagating across connecting chambers.
- Flammability and extinction measurements including the role of water droplets, showing droplets can serve as wakes to flames, leading to acceleration rather than suppression.
- Interesting insights developed into the monitoring and passive mitigation of accidents during and after the development of the accident with loss of power – how to power these devices intrinsically, which is the topic of MITHYGENE project: passive sensor in nuclear power plants.
- Behaviour of combustion between magnesium and aluminium powders.

The published studies range from the very fundamental to the very applied, but always using the state of the art tools appropriate for understanding the particular characteristics.

Importantly, the current grant has served to develop the fundamental tools to understand the overall characteristics of the processes, whilst carrying over the results to the more applied industrial realm.

Recommendations: these are impressive studies, unlikely to be easily reproduced elsewhere, and making excellent use not only of the existing Labex facilities, but also of combined international facilities and expertise.

Inter LABEX Activities

The committee appreciated the three joint research projects between CAPRYSSES and VOLTAIRE labex. They open new opportunities of collaborations on the campus of Orléans between research units from separate domains but working on gases/volatiles, viewed from either an Energy or Earth Sciences perspective: this potentially represents a very good case of cross fertilization between disciplines. In general, the committee notes that, whereas the sharing of technical expertise and use of (often unique) laboratory facilities is a great asset for the proposed activities, the scientific questions underlying the planed laboratory efforts have not been not well shown and require to be better expressed or defined. Overall, the committee recommends apprehending these future actions progressively, in a step-by-step approach, to make sure that this block of new actions does not drive CAPRYSSES activities away from its well-established core of expertises in the Energy field.

In detail, questions raised during the presentation and during the committee meeting can be summarised as follows:

Hydrochar: although it is clear that the use of biomass as an alternative energy source requires further experimental investigations, the role of Earth Sciences players need to be better defined in the project, which gives so far an account of past efforts in the domain by ICARE... The complementary knowledge gained from either BRGM (French Geological Survey) or ISTO would benefit from being explicitly written.... Is the soil amendment activity relevant for an inter-Labex project? What could be the contribution of Caprysses on this theme?

Volcanic gases: The committee sees this research topic as an important occasion to disentangle the physico-chemical processes occurring during mixing between volcanic gases and atmosphere. As expressed before, the question as to why carrying out such a program needs to better spell out, in particular in terms of its global significance. The committee welcomes the modelling efforts, which include an explicit treatment of kinetics aspects. The committee recommends however that 2-3D modelling be planned as well, so as to look at the fluid dynamics of hot volcanic jets into the atmosphere, and understand properly the geometry of mixing and related chemical processes. It also encourages to carry out in parallel the experimental simulation of the studied processes, for which ICARE facilities are well adapted to, and which could provide important data to test/calibrate the models. Why not involve the atmosphere chemistry team of ICARE, today outside of the Caprysses perimeter, in this activity?

Atmospheric entry: The committee also considers this research topic of considerable interest. The reason why undertaking such an ambitious laboratory work remains, however, to be refined. Labex VOLTAIRE is interested in looking at the role and fate of natural volatiles issued from Earth: its interest on stratospheric phenomena has been focused on characterising aerosols and understanding their origin, owing to their role on global climate. In such a context, the experimental simulation (using the unique ICARE facilities) of meteorites survival/behavior during atmospheric entry may potentially shed a new light on aerosol's origin in the stratosphere. In contrast, the research activity concerning the origin of life, while interesting per se, does not represent the main scientific targets of either CAPRYSSES or VOLTAIRE labex, and its funding should perhaps be considered elsewhere, in order to keep Labex's research focused.

Labex CAPRYSSES Review Committee Members:

Prof. Robert Dibble, University of California Berkeley, USA and KAUST, Saudi Arabia
Prof. Simone Hochgreb, University of Cambridge, UK
Prof. Jonathan Morrison, Imperial College, UK
Prof. Heinz Pitsch, University of Aachen, Germany
Dr. Bruno Scaillet, Labex Voltaire, France
Dr. Denis Veynante, CNRS-INSIS, EM2C, France