Accounting for soot particle morphology in flame thermal radiation and optical diagnostics in complex systems

Summary table of persons involved in the project:

Partner	Name	First name	Current position	Role & responsibilities in the project (4 lines max)	PM	Tasks		
CERFACS	*Riber*	*Eleonore*	*Researcher*	*Coordinator Modelling of PM particle production Responsible for analysis and comparison of the results in the MICADO burner*	*12*	X		X
			PhD	*Modelling of PM particle production and coupled simulation of the MICADO combustor*	*36*	X		X
	Misdariis	*Antony*	*Researcher*	*Improvement of PRISSMA radiation solver and coupled simulation of the MICADO combustor*	*3*		X	X
	Vermorel	*Olivier*	*Researcher*	*Integration and validation of PM model in AVBP*	*1*	X		
CORIA	*Yon*	*Jérome*	*Associate professor*	*Responsible of the aggregates generation and radiative properties determination*	*12*	X	X	X
	Roze	*Claude*	*Professor*	*Particle-light interaction*	*3.4*		X	
	Poux	*Alexandre*	*Engineer*	*DLCA code development*	*4.8*	X		
			PhD	*DLCA code development and soot radiative properties*	*36*	X	X	X
ONERA	*Gaffié*	*Daniel*	*Engineer*	*Technical coordination of ONERA tasks*	*3.5*	X		X
	Dellinger	*Nicolas*	*PhD*	*Reduced gas chemistry*	*6,4*	X		X
	Boucher	*Aymeric*	*Engineer*	*Numerical simulation of sooting flames*	*5,6*	X		X
	Vincent	*Axel*	*Engineer*	*Measurement campaign on MICADO set-up*	*5,5*			X
RAPSODEE	*El Hafi*	*Mouna*	*Associate professor*	*Radiative transfer modelling by statistical approach*	*6*		X	X
			PostDoc	*Modelling (scattering and UQ in MCM3D, production of a digital image)*	*12*		X	X
			Subcontracting PostDoc	*IT engineering to develop MCM3D code and produce a digital image of the flame*	*12*		X	X

Any changes that have been made in the full proposal compared to the pre-proposal

Following the recommendations of the pre-proposal reviewers to better link WP2.3 to the rest of the project, an experimental campaign of measurement of planar light scattering by soot (WP3.2) has been added to the original proposal. This campaign induces an additional cost of 45 keuros, increasing the budget of the project by 9% compared to the initial proposal.

I. Proposal's context, positioning and objective(s)

a. Objectives and scientific hypotheses

To answer the increasing needs of our modern society, combustion remains a major source of energy. Other solutions including, but not limited to, the ongoing integration of renewable energy sources (solar, wind, geothermal, etc.), and in some countries the nuclear energy, are expected to be versatile and may also be associated to combustion systems. Combustion is however associated to hazardous effects on human health and to unprecedented concerns on global warming and climate change due to ultrafine particulate matter (PM) and other pollutants emissions. Numerous epidemiological studies over the past decade have concluded that exposure to ultra-fine particulates (nanometer sized, like soot particles) increases mortality due to their deep penetration into vital human organs, such as heart and lung, thus causing severe diseases associated with these organs. Soot particles also affect the Earth's temperature and climate by altering the radiative properties of the atmosphere and current estimates put soot particles, also called black carbon in aerosol and climate sciences, as the second largest anthropogenic contributor to climate change, just after carbon dioxide (CO2). Unlike CO2 however, soot particles have a fairly short life span in the atmosphere, of the order of few weeks. Consequently, it is suggested that a reduction of soot emissions from combustion systems and vehicles is an effective and rapid mean to slow down global warming and climate change. All these concerns have led to strongly strengthen regulations on exhaust emissions from combustion devices. The reduction of soot emissions by combustion devices is a particularly difficult challenge, due to the complexity of the involved mechanisms but also because in some cases, such as in boilers and furnaces, soot particles contribute to the system efficiency thanks to their significant enhancement of radiant heat transfer.

To optimize current industrial designs and develop new ones with significant reduction of PM emissions, accurate prediction tools in real configurations are needed. This first requires to better understand the complex underlying physical mechanisms of PM formation. Many experimental studies are reported in the literature, where PM are characterized in terms of number density and size at the exhaust of combustion systems (refs). Measurements of PM inside burners, which give a better insight into PM processes, are more difficult and more scarce (Geigle *et al.* 2015). Going into even more details, soot morphology has been characterized experimentally and shown to play a critical role on PM formation processes. As a complement to experiment, and the only prediction tool for industrial design, Computational Fluid Dynamics (CFD) has become a powerful and essential technique, benefiting from both the improvement of modelling accuracy and the continuous growth of computing power. CFD not only gives a detailed insight on the resolved physical processes, but is today able to accurately predict many unsteady features of combustion systems by employing the Large Eddy Simulation (LES) approach (Gicquel et al. 2012, Jourdaine et al. 2017). This is however not yet the case for PM emissions, which is the topic of intense current research. Predicting PM emission is a complex multi-physics problem, including heterogeneous chemistry and thermal radiation that must be taken into account. Both require a good description of the PM size, but are also sensitive to the PM shape and composition. Such details about the particle morphology have never been included in PM emission CFD models due to the induced complexity. Today however, the available computing power allows to revisit these models in a way that significantly facilitates the detailed description of PM. **This is the global objective of ASTORIA**.

Modelling PM formation and transport in CFD of complex geometries is particularly challenging for three main reasons. First, the gas phase chemistry which produces burnt gases including PM precursors (PAHs) and radical species plays a key role in the PM formation through nucleation, condensation and surface reaction processes. Today, most studies dealing with PM formation use either tabulation methods which assume a flame structure (either premixed or diffusion) that is not representative of the real flame (Rodriguez et al. 2017), or a reduced chemistry which does not include all the PAHs required to properly reproduce PM production. Second, an accurate numerical approach must be used to correctly reproduce PM volume fraction, particle-size distribution (PSD) and other particles properties (such as shape). Today, the PSD in practical systems is solved either with sectional approaches (SM) (Saggesse et al. 2015) or methods of moments (MOM) (Mueller and Pitsch 2013). Such methods require specific numerical schemes and their cost increases drastically with the number of soot properties to be described, explaining why they do not take into account PM morphology. Finally, as PM are thermally radiative, their radiation properties must be correctly described as functions of their morphology and composition. Indeed, assuming a spherical shape as is done nowadays in most CFD and thermal radiation soot models (in order to use the Mie theory), can lead eventually to large errors. Moreover, this simplification limits the possibility of comparison with experiments based on laser diagnostics.

In order to evaluate the radiative properties of PM by taking into account their morphology, the aggregates have first to be described as virtually conceived particles (Ceolato et al. 2013; Yon et al. 2014). The reference method currently used for this PM generation is the Diffusion Limited Cluster-Cluster Aggregation (DLCCA), simulating the 3D Brownian motion of primary spheres and their collisions, each collision event leading to the formation of an aggregate. Unfortunately the application of such approach usually misses some important physics (temperature is not considered as well as a physical residence time). Moreover, surface growth and the consequent overlapping of primary spheres are not considered. Only few studies attempted to evaluate the impact of a realistic morphology on the radiative properties of PM (Okyay and Enguehard 2014, Yon et al. 2015a). These studies all considered only individual radiative properties of particles (cross sections). However in dense and inhomogeneous particle populations such as those found in real combustors, multiple scattering between particles occur. This has a direct impact on the total thermal radiation of the flame. It may also significantly alter optical diagnostics widely used for flame measurements.

To progress beyond the current state-of-the-art of our understanding of PM emissions, and to improve CFD capabilities for their prediction in real configurations, a combined approach is required in multiphysics simulations associating turbulence, combustion and soot gaseous chemistry, PM formation and evolution as well as thermal radiation with morphology-based soot radiative properties.

Therefore, the main objectives of ASTORIA are to (i) propose an alternative to SM and MOM allowing to compute the evolution of the PM population and properties, including morphology and a detailed gaseous chemistry; (ii) develop a new physically-based DLCA approach for aggregate generation, taking into account physical local conditions along particle trajectories, (iii) produce radiative properties in the infrared range accounting for soot aggregates morphology. All these new model developments will be integrated in a CFD code to improve the prediction of emitted PM number and shape in industrial applications, which is the global objective of ASTORIA.

Such developments will also allow to compute radiation in the visible frequency range, in order to reproduce numerically laser-based diagnostics such as static light scattering, line of sight extinction or laser induced incandescence. This will pave the way to a more direct comparison between simulations and experiments for a better understanding and prediction of PM emission. The improved knowledge and description of soot radiative properties will also increase the accuracy of laser-based diagnostics and climate models.

The methodology proposed in **ASTORIA** requires a strong expertise in high fidelity numerical approach of sooting flames in complex geometries, DLCA approach for aggregate generation and accurate radiation simulation of both the burnt gases released by combustion and the soot aggregates. To the best of our knowledge, such coupled simulations have never been performed and give to the **ASTORIA** project significant originality and innovation in comparison with other current projects in the field.

b. Originality and relevance in relation to the state of the art

A first originality of this project is to propose an alternative to SM and MOM to compute the evolution of the soot particle population and their morphology in practical systems. Indeed, SM and MOM approaches would require to significantly increase the number of sections or moments to represent soot particle shape. Only Lagrangian-based methods are able to easily include additional particle properties. This is the case for Monte-Carlo (MC) approaches, performing a Lagrangian tracking of *stochastic particles*. MC however requires to compute a very large number of particles to reach statistical convergence, and requires to model stochastic processes. It the present project, a semi-deterministic Lagrangian approach is proposed, where trajectories of *physical particles* are computed. The innovative aspect of the method relies in the fact that not all physical particles are computed, but only a subset of representative particles that are possibly present in a control volume. Collisions are then treated via stochastic processes. This allows to drastically decrease the computational cost and make the approach affordable for soot prediction in complex geometries. As such it makes an optimum trade-off between computing cost and accuracy. This requires however an efficient parallel algorithm for the calculation of Lagrangian particles, as well as a careful control of statistical convergence of the representative particle subset. **To our knowledge such approach has never been published for soot prediction in real systems.** The reason is to be found in the prohibitive computational cost of the Lagrangian calculation of all physical particles in a 3D configuration. Both the progress made in parallel computing of turbulent spray flames using AVBP (Gourdain *et al.,* 2009) and the semi-deterministic concept described above allow to overcome this issue in the present project.

Soot chemistry requires detailed chemical kinetic mechanisms which allow a comprehensive description of the intermediate species and soot precursors in the gas phase. Their direct integration is however prohibitive from the point of view of computational and memory requirements. As part of the **ASTORIA** project, we are moving towards the use of less expensive reduced reaction mechanisms which remain coupled to particle size and nonsphericity. Such reduced mechanism will be developed for a realistic aviation fuel (Jet A1), as none is currently available in the literature.

A second originality of the present work concerns the generation of virtual aggregates. First, the proposed approach is able to consider the impact of the local thermodynamic conditions, surface growth and oxidation of the particles during the aggregation processes. This is done by introducing a physical residence time. Second, the aggregate generation is coupled with CFD flames simulations in order to constrain the virtual generation of aggregates with the evolving physical environment seen by the particles during their formation. This represents the most important advance regarding the generation of virtual aggregates proposed by the present project. Pertinent parameters for the soot formation will be computed along Lagrangian pathways extracted from the CFD simulations, and expressed as functions of the residence time, enabling the simulation of growth and agglomeration by the developed physical DLCA code. Thanks to this innovative approach, we expect to produce aggregates with a primary particle size distribution, degree of overlapping and number of primary spheres representative of the soot particles encountered in the simulated flames.

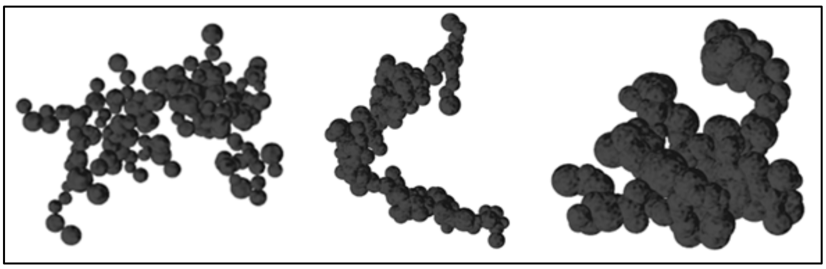


Figure 1: *Examples of aggregates generated by the DLCA code (CORIA) with different scenarios of surface growth*

The third originality of the proposed project concerns the determination of the radiative properties of soot particles. Radiative properties depend on the morphological specificity of the particles (fractal aggregates), their variable size (for aggregates or for their primary spherules) and the variability of their optical index with wavelength. A simple analytical model called RDG-FA (R.A. Dobbins and C.M. Megaridis, 1987) enables the determination of scattering and absorption cross sections of fractal aggregates. Nevertheless, the underlying theoretical assumptions make the obtained cross sections inaccurate. For example, multiple scattering occurring or the interpenetration of the primary spheres (overlapping) can not be taken into account. In order to describe the complex light interactions occurring in the particles, the solving of the Maxwell equations is required. For simple geometries (just touching spheres), T-Matrix methods may be used. However the only method that currently enables the rigorous determination of the radiative properties for complex particles shapes is based on the dipolar approximation (DDA). Only few studies attempted to evaluate the impact of a realistic morphology on particle radiative properties (Bescond et al., 2013; Okyay & Enguehard, 2014; Yon et al., 2015; Doner et al., 2017), and they consider only individual radiative properties (cross sections). In the present work, the Maxwell equations will be numerically resolved to describe the light interaction with particles for the particles previously obtained with DLCA along Lagrangian pathways of the CFD simulation. This will allow to determine the radiative properties of realistic soot particles as functions of their aging in the flame. Because the computing cost is high for each studied aggregate, the radiative properties will be evaluated for a set of representative particles all along the simulated flames. This methodology will ensure a determination of the radiative properties of individual aggregates as functions of their position in the simulated flames. If some general trends appear, we will try to interpret the results in terms of general correction laws for the RDG-FA theory. Indeed, a corrected RDG-FA approach would be simpler to implement and use in the solving of the radiative transfer equation, and as such would represent a significant innovation in the field.

Finally, a fourth originality is the computation of a digital image of the flame. **ASTORIA** will take advantage of new algorithms based on null collision (Galtier et al. 2013). The strict orthogonality between the statistical algorithm and data-representation allows a significant reduction of the CPU cost. This independence of data-representation enables the implementation of acceleration grids (M. Pharr and G. Humphreys, 2010). This issue has been addressed by the computer graphics community (Kutz *et al.* 2017) who used the algorithms developed by RAPSODEE to get both a high resolution imaging and a fast rendering. As uncertainty quantification is also an interesting feature of this approach, the sensitivities will be provided without additional computational cost.

c. Methodology and risk management

To reach its ambitious objectives, the **ASTORIA** project proposes to focus on the development and improvement of numerical tools, and to mainly rely on existing measurements for validation purposes. The only experimental work that is part of **ASTORIA** is the measurement of planar light scattering by soot, required to validate the computation of a digital flame image. Data will be otherwise taken from three experiments that address specific topics relevant to **ASTORIA**:

- The Laser-Induced Incandescence (LII) database provided by the LII Workshop (http://liiscience.org/target_flames) provides extended data to characterise the flame and the soot production in academic ethylene-air laminar premixed and turbulent jet sooting flames.
- The ISF3-Target Flame 3 is a non-premixed swirled ethylene-air burner installed at DLR (Geigle *et al.* 2015) (*Figure 2*a. and b.) specifically designed to study soot in gas turbine combustors under elevated pressure. It is one of the reference complex configurations for soot modelling within the International Sooting Flame (ISF) workshop and is also studied within the H2020 SOPRANO project (2016-2020). It operates at two pressures (3 and 5 bars) and at a global equivalence ratio Φ=0.86. Several laser diagnostics are available for each operating point : Stereo - Particle Image Velocimetry (S-PIV) for velocity, Coherent Anti-Stokes Raman scattering (CARS) for temperature, Laser Induced Fluorescence for a qualitative estimate of the OH radical distribution, and Laser-Induced Incandescence (LII) for soot volume fraction. Both CERFACS and ONERA

have computed the ISF3 configuration prior to **ASTORIA** using a reduced ethylene-air chemistry for the gas phase and a Lagrangian deterministic tracking for soot particles (Gallen *et al.* 2018, Dellinger et al. 2017).

- The MICADO test rig, located in ONERA Palaiseau has been recently developed to study multiphysics combustion processes, at high pressure and high temperature, in conditions representative of real aero-engines. The combustor is in size comparable to a real engine single-sector. It is fed with air and kerosene by an axial single-swirl injector, the fuel being injected through the main and/or pilot supplies, leading to various turbulent combustion regimes. Thanks to large optical accesses, a huge database is being acquired within the SOPRANO project, using laser-based, optical and conventional diagnostics (PIV, OH*/CH* chemiluminescence, CARS, and LII for soot volume fraction), and exhaust gases sampling. The MICADO test rig aims at helping to consolidate multiphysics codes and model, and bringing advanced experimental techniques to a higher TRL level. In the framework of **ASTORIA**, an additional campaign focused on the determination of light scattering patterns in the visible domain will be conducted at ONERA in collaboration with CORIA.

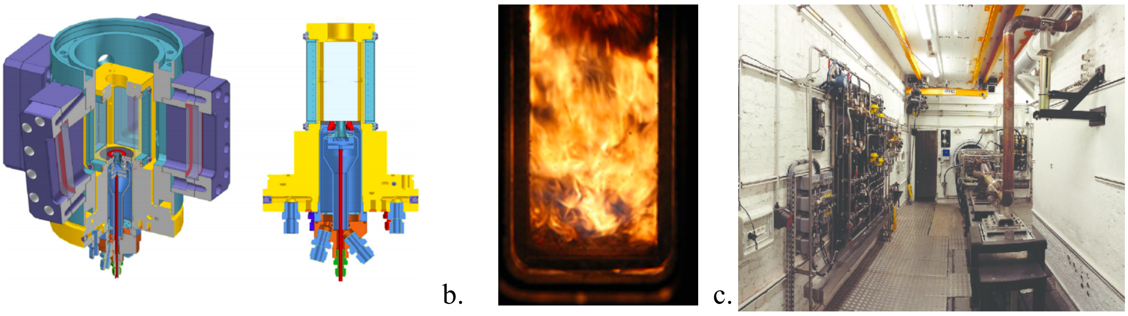
a. b. c.


*Figure 2: Configurations studied during the **ASTORIA** project: ISF3-Target Flame 3 burner (a.), photo of a sooting flame in ISF3-Target Flame 3 (b.), and MICADO test-rig (c.)*

To reach the project objectives, the work is structured in 4 Work Packages, as shown in *Figure 3*:

- **WP0 ensures the successful management of the project**, its coordination as well as the dissemination and exploitation of the results.
- **WP1 is devoted to the numerical simulation of sooting flames in complex geometries and the modelling of the morphology of soot aggregates**. The LII database and the ISF3-Target Flame 3, already studied numerically by CERFACS and ONERA within the ANR SMARTLECT, but using a simplified model for the gaseous chemistry and a semi-empirical soot model, will be used in this WP. ONERA will first use reduction tools to provide an accurate description of the gaseous ethylene-air chemistry, including an accurate description of the PAH soot precursors (WP1.1). The reduced chemical model will be implemented in the CEDRE multi-physics platform of ONERA for evaluation in the ISF3-Target Flame 3. ONERA will then apply the same methodology to jetA1-air flames to be used in WP3. In WP1.2, CERFACS will develop the Lagrangian semi-deterministic approach for the simulation of soot particle dynamics and evolution. This will be done in the AVBP solver, extensively used for turbulent combustion simulation in academic as well as complex real geometries. The reduced chemistry developed in WP1.1 by ONERA will be also implemented in AVBP, to simulate the academic ethylene-air flames of the LII database without thermal radiation. Specific post-processing will be implemented in AVBP to record the thermodynamic histories of the particles travelling in the burner. Those will be used in WP1.3 by CORIA to develop a new physically-based DLCA approach for aggregate generation, using physical local conditions along particle trajectories.
- **WP2 focuses on the numerical simulation of radiation, both in the infrared and the visible frequency ranges.** Based on the virtual aggregates generated in WP1.3, CORIA will evaluate in WP2.1 the particle radiative properties in the infrared and visible domain by solving the light-particle interaction electromagnetic problem with the use of the DDSCAT code (Draine and

Flatau, 2013). In WP2.2, RAPSODEE and CERFACS will implement these particle radiative properties in two radiation solvers: the code PRISSMA of CERFACS solves the Radiation Transfer Equation using a Discrete Ordinates Method while the open-source code MCM3D of RAPSODEE provides reference solutions for the radiative heat transfer. Coupled combustion/radiation simulations using AVBP and PRISSMA will be performed in the LII database and the ISF3-Target Flame 3 configurations. Finally in WP2.3, RAPSODEE will develop a numerical approach to compute a digital image of the flame in the visible domain.

- **WP3 aims at applying all the numerical methods developed in WP1 and WP2 to the MICADO kerosene-air combustor.** First in WP3.1, CERFACS will perform a coupled combustion/radiation simulation including the developments of WP1, WP2.1 and WP2.2. WP3.2 is devoted to the computation and validation of radiation of sooting flames in the visible domain. In WP3.2.1, measurement of planar light scattering by soot will be conducted by CORIA and ONERA. In WP3.2.2, RAPSODEE will apply the numerical method developed in WP2.3 to compute the digital image of the flame at the same operating points. WP3.3 finally aims at performing. a detailed analysis and comparison of the experimental and numerical results in terms of sooting flame structure and radiation in the infrared and visible domains.

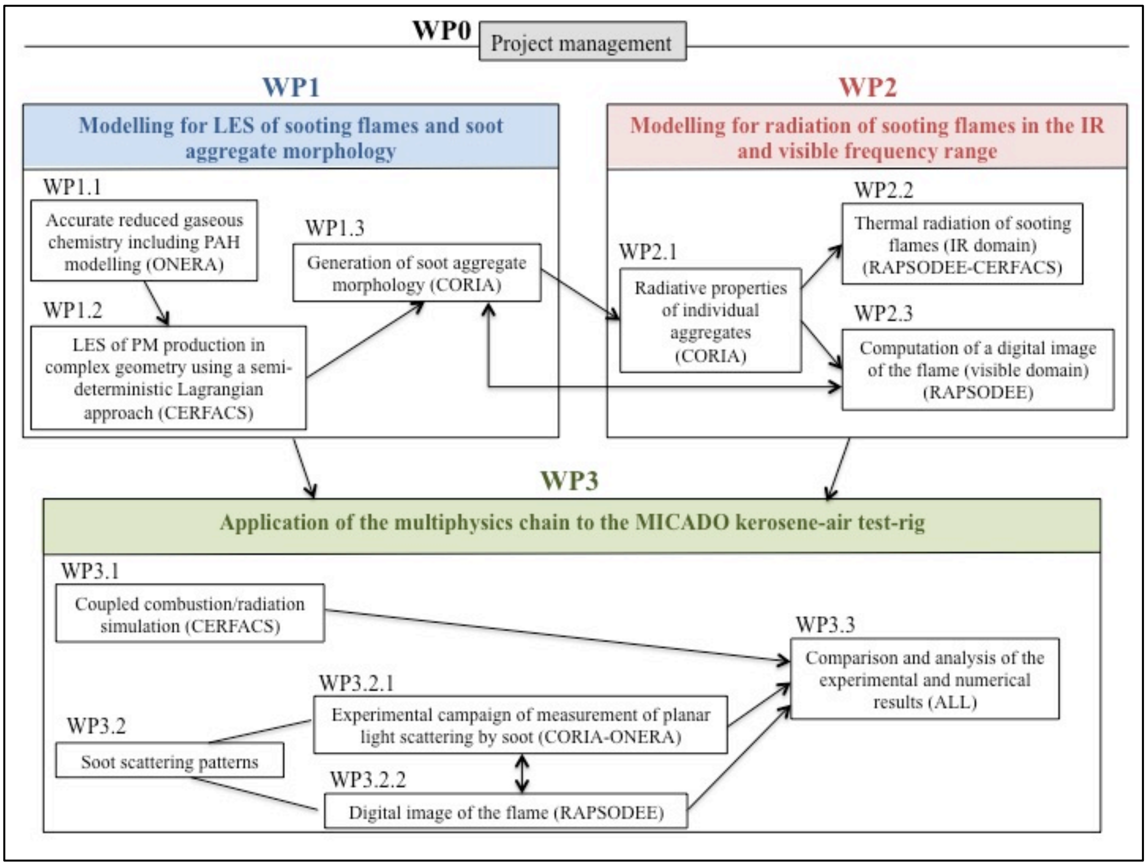


Figure 3: Project organisation

<u>**Description of the codes used in ASTORIA**</u>

- **AVBP** is co-developed by CERFACS and IFPEN since 1993. It is a parallel explicit CFD code that solves the turbulent reactive compressible Navier-Stokes equations on massive unstructured and hybrid grids using LES. To account for liquid fuel, a classical Euler-Lagrange approach is used. Tabulated chemistry (Gicquel et al., 2000) or Analytically Reduced Chemistry (Jaravel *et al. 2017,* Felden *et al. 2017)* allows studying combustion, coupled with turbulence-combustion models (Colin et al., 2000a, Fiorina et al., 2010). The AVBP software is part of the PRACE benchmarking suite and has been validated for a large range of applications. AVBP is distributed for "open science" projects to a wide range of research entities in Europe and in the world. (EM2C-CNRS, IMFT, CORIA, Université de Pau, Technical University of Munich (Germany), CIEMAT (Spain), University of Sherbrooke (Canada). Several industrial companies (SAFRAN, TOTAL, RSA, PSA, ALSTOM, ANSALDO, AIR LIQUIDE, GDF…) have access to AVBP and benefit regularly from the different developments in the code.

- **CEDRE** is a multi-physics platform developed at ONERA, for both research and industrial applications, in the fields of energetics and propulsion. The software architecture follows a multi-domain, multi-solver approach for gas phase, dispersed phase, thermal fields in solids and radiation. These solvers share the CEDRE architecture and libraries, and can be coupled. Computations cover the fields of aerodynamics, aerothermal coupling (heat transfer), combustion, water ingestion, icing, propulsion, and aeroacoustics.
- **DDSCAT** is used for the evaluation of the radiative properties of individual aggregates. It relies on the Discret Dipole Approximation that consists in the decomposition of the particle generated by the DLCA code in a large number of individual dipoles who interact with the light. DDSCAT is a free code developed by Drain and Flateau, 2013 that presents the advantage over other existing codes as T-Matrix to enable the evaluation of the radiative properties (absorption and scattering cross sections) for any desired complexes shapes. The CORIA has a long experience in using that code in order to determine the exact radiative properties of soot. The effect of the primary sphere, number of primary spheres and wavelength, necking and overlapping, coating have been studied by our group using DDSCAT. The results obtained by this code have been satisfactorily compared with other numerical approaches in the context of international benchmarks and collaborations (Ch. Sorensen's group in US, F. Liu in Canada). In case of systematic evaluation of many aggregates and for several wavelengths, DDSCAT can be used in parallel version and executed on computational centers as on Myria at Criann (Normandy calculation center).
- The **DLCA** code is developed since 2009 at CORIA laboratory, initially in the framework of a collaboration with IRSN [5]. It consists in simulating the Brownian motion of primary spheres and aggregates caused by the local temperature and by considering their size and mass in order to simulate their aggregation caused by their respective collisions. The DLCA code development has been regularly pursued by H. El Gueddari (L3 in 2012), during the PhD of A. Bescond (2013-2015). More recently, first implementations of the surface growth of the primary spheres and of the coupling with extraction pathways from CFD codes have been successfully tested during the master 2 traineeship of A. Simeon (2016). The investigation of implementing fragmentation is currently under investigation by a M2 traineeship (O. Belhri, 2018). Also, efficiency of the code architecture has been improved during the traineeship of E. Menier (L2, 2017). In consequence of this historical experience, there are no significant risk associated to the development of that code and its coupling with partners's CFD (see description of the task WP1.2.
- **MCM3D** allows to provide radiative transfer term source and wall fluxes taking into account gas (k-distribution approach) and soot radiation. It is open-source and will be documented and distributed to the community via the EDStar platform (http://edstar.lmd.jussieu.fr/). In the next two years, the platform will be extended with a set of e-learning tools concerning statistical-engineering of complex systems (project Contrat de collaboration Laboratoire-Entreprise, CLE-2016, supported by the région Occitanie).
- **PRISSMA** (CERFACS) is a Radiative Transfert Equation (RTE) solver based on the Discrete Ordinates Method (DOM) for unstructured hybrid meshes. It has been developped within several ANR (CORAYL, SMARTLECT) and FNRAE (STRASS) projects. The solver is able to treat industrial geometries (with a high number of cells > 1 milions) and uses an angular discretisation as well asdifferent spectral models : simple gray gas, WSGG, FS-SNBcK and SNBcK.

Risks & Contingency plans

WP	Risk	Probability	Fall-back solution
WP1	Difficulties in numerical model development and validation.	Low	Use of simplified models for the gaseous chemistry of PAHs from the literature
	Difficulties to select representative species of soot oxidation and surface growth from CFD simulations for a correct simulation of aggregate size and morphology with the DLCA code.	Certain	Some adjustments have to be performed through macroscopic unknown parameters as accumulation parameters for example.
	Lack of precision of the models developed for high pressure combustion conditions (a key question of the **ASTORIA** project)	Certain	In-depth investigation of the experimental-numerical comparison. Implementation of a sensitivity study for different pressure level from moderate (5 bar) to high pressure levels (20 bar) in order to calibrate the models, accordingly.
WP2	Selection of optical indices used for the evaluation of the soot radiative properties.	Certain	Apply recent advances recently published on that topics. Different scenarios can be considered.
WP3	Difficulty in performing an appropriate experimental-numerical comparison to allow a relevant validation of advanced models developed in WP1 and WP2	Medium	Change of operating point of MICADO for a less demanding case.

II. Project organisation and means implemented

a. Scientific coordinator and its consortium / its team

The consortium gathers partners with specific expertise in CFD of reacting flows in complex geometries, physical modelling of PM formation and subsequent particle aggregates as well as radiation and multi-physics.

CERFACS is a research organization developing advanced methods for the high-fidelity numerical simulation of large scientific and technological problems of interest for research and industry.
Dr E. Riber, senior researcher highly experienced in LES of turbulent combustion in complex geometries and modelling of pollutant emissions will coordinate the project. She graduated from ENSEEIHT in 2003 and then worked at IMFT and CERFACS in the field of two-phase flow modelling to obtain her PhD from INPT in 2007. After one year as a researcher at IFPEN, she joined CERFACS in 2008. She has now more than 25 papers in referred journals. She coordinated the STRASS project supported by FNRAE (2009-2012) and is currently involved in two ANR (NEXTFLAME, TIMBER) both finishing in 2018 and 3 European projects (SOPRANO, JETSCREEN, IMPROOF).

CORIA is a mixt academic research center (CNRS-INSIS, University and INSA of Rouen) specialized in the numerical and experimental investigation of reactive and non-reactive flows. CORIA has a strong expertise in the development of laser based techniques for in-situ characterization of flames and sprays. Dr J. Yon, participant of the project, is assistant professor since 2004. He is expert in soot characterization by optically based techniques and non-optical techniques. He has also a strong numerical and theoretical activity concerned by the generation of virtual aggregates and the determination of their radiative properties. He obtained the habilitation to conduct researches in 2014 at Rouen University. He has already coordinated different projects including one founded by the LABEX EMC3 and another one by Carnot ESP. He participated to 23 national and European projects. He is author or co-author of 33 papers in international refereed journals.

RAPSODEE is centered on product oriented process engineering and involves a radiative team working in the field of planetary atmospheres, combustion and concentrated solar energy. RAPSODEE is also a laboratory of excellence (SOLSTICE http://rapsodee.mines-albi.fr/en/co/SOLSTICE.html). As a specialist of radiation simulation, M. El Hafi, assistant professor, will be the scientist in charge for this project. She focuses on the statistical approaches to complex-systems for combustion, solar energy, photobioreactors and atmospheric applications. She also animates the axis "transferts couplés" of the GDR CNRS ACCORT federating thermal radiation at the research at the national scale (http://www.gdr-accort.cnrs.fr), 35 publications in peer-reviewed international journals.

ONERA, Dr. D. Gaffié, expert engineer in the field of modelling and numerical simulation of turbulent and reactive flows, will participate to the project. He has led and participated in recent research projects related to soot formation in combustors, their influence on radiative transfers and the measurements of gaseous and PM emissions linked to OACI regulation of civil aviation.
All partners know each other well and have already nourished fruitful collaborations in preceding ANR (CORAYL, STRASS, SMARTLECT), DGA project (MERMOSE) and European (FIRST, SOPRANO, JETSCREEN) projects.

b. Means of achieving the objectives

- **WP0 - Project management (Leader CERFACS)**

Leader: CERFACS	Partners: All	Start / End: M0 / M48
Objectives	Coordination of the project. Organization, management, follow-up, reporting, dissemination, advertisement and exloitation.	
Work Programme	**WP 0.1**: Consortium Agreement **WP 0.2**: Project management **WP 0.3**: Project meetings and Reporting **WP 0.4**: Collection and Quality Assessment of Deliverables **WP 0.5**: Project advertisement and promotion **WP 0.6**: Dissemination and exploitation of results	
Deliverables	D0.1: Minutes of meetings (CERFACS, periodic) D0.1: Mid-term report (CERFACS, M24) D0.2: Final report (CERFACS, M48)	

This task ensures the successful management of the project, on the scientific and technical levels and in terms of administration, reporting and contractual matters.

WP 0.1: Consortium Agreement
A Consortium Agreement will be prepared and proposed to all partners for signature. The document will specify the rules for collaboration and exchange of data, knowledge and software. The following points will be addressed:
- Common property of the results is shared by the partners who have contributed to the work.
- In the event of exploitation of the results, the amount of the respective contributions established by the financial annex may be used to determine property quota shares and to negotiate royalty amounts.
- The right for publication is preserved for all researchers.

WP 0.2: Project management
The project management will be performed by the coordinator, with the help of a **Management Committee** composed of one representative per partner, who will locally organize the project implementation at their respective institution. The PhD and postdoc positions will be advertised by all partners, but the recruitment will be made by each partner independently. The Management Committee will define the rules for an efficient project implementation and progress.
If necessary, the Management Committee will also take decisions concerning possible modifications of the project planning or objectives. In case of conflict or disagreement, the coordinator will take the role of mediator to reach a consensus.
Specific means will be set-up for the exchange of data and possibly software, via dedicated internet platforms with restricted access.

WP 0.3: Project meetings and Reporting
Regular meetings will be organized every 6 months. The first and last meetings will be organized at CERFACS and the other meetings will be organized in partner labs. The coordinator will take and distribute the minutes of each meeting.
Additional meetings between two partners collaborating in a WP will be organized on demand by the concerned partners. Those will also take minutes and distribute them to the Consortium for information.
The coordinator will be responsible for intermediate and final reporting to the ANR. He will also collect and present the project implementation and results at the mid-term review meeting.

WP 0.4: Collection and Quality Assessment of Deliverables
The coordinator will collect the Deliverables when they are due according to the project planning. In case of delay, a new delivery date will be agreed on with Management Committee and the partner responsible of the Deliverable, taking into account the reasons for the delay and making sure that it does not impact the progress of other tasks.
In order to ensure a good quality, each Deliverable report will be reviewed by a partner of the project who has not contributed to the report, and assigned by the Management Committee. The reviewer will then interact with the authors of the Deliverable to propose possible improvements.

WP 0.5: Project advertisement and promotion
Several means will be used and set-up by the coordinator to advertise the project and promote its activities:
- A web-site, with unrestricted access to the public, presenting the project and major achievements
- Posters and leaflets to be presented and distributed at conferences or meetings
- Announcements of open positions which will be largely distributed, through networks such as for example the Groupement Français de Combustion (GFC)
- Writing of articles for popularizing journals, or book chapters for students.

WP 0.6: Dissemination and exploitation of results
The coordinator will be responsible for these Tasks described in the Impact section.

- **WP1: Modelling of particle morphology in complex reacting flows**

Leader: CERFACS	Partners: CERFACS, CORIA, ONERA	Start / End: M0 / M24
Main objective	Modelling for LES of sooting flames and soot aggregate morphology	
Work Programme	**WP 1.1**: Accurate reduced gaseous chemistry including PAH modelling (ONERA) **WP 1.2**: LES of PM production in complex geometry using a semi-deterministic Lagrangian approach (CERFACS) **WP 1.3**: Generation of soot aggregate morphology (CORIA-CERFACS)	

Deliverables	D1.1: Gas phase chemistry for jetA-1 combustion including PAH (ONERA, M12) D1.2: Semi-deterministic Lagrangian approach for PM production (CERFACS, M24) D1.3: Advances in the generation of virtual aggregates with realistic morphologies (CORIA, M24)

The objective of WP1 is to develop a numerical method to perform numerical simulations of PM production in complex geometries including complex gas phase chemistry and PM size distribution, and to couple it to a DLCA method able to generate the morphology of particle aggregates.

#WP1.1: **Accurate reduced gaseous chemistry including PAH modelling (ONERA)**
The PM formation through nucleation, condensation and surface reaction processes strongly depends on the gas phase chemistry which produces burnt gases including PM precursors (PAH) and radical species. Whereas many studies dealing with PM formation rely on tabulation methods which assume a flame structure (either premixed or diffusion) that is not representative of the real flame (Rodriguez et al. 2017), CERFACS has shown the capacity of Analytical Reduced Chemistry to correctly reproduce the complex flame structure as well as acetylene which is one classical PAH used in the literature. To increase the level of accuracy of such approach, larger PAH must be taken into account. Following the work of Eberle *et al., 2017* the reduced mechanism they proposed (43 species, 304 reactions) will be further reduced using classical (partial equilibrium analysis) or more innovative (genetic algorithms) reduction techniques. Moreover, the reactions governing the evolution of PAHs and their radicals until nascent soot particles, will be modelled using the sectional approach proposed in the work of Eberle *et al.*, 2017, and coupled with the reduced gas-phase mechanism. Such a modelling approach will be implemented in the CEDRE solver from ONERA, validated first in canonical flames and then in the ISF3-Target Flame3 configuration from DLR. Finally, a reduced chemistry will be derived for Jet-A1-air flames following the same methodology, to be used by CERFACS in the LES of the MICADO test rig using AVBP.

#WP1.2: LES of PM production in complex geometry using a semi-deterministic Lagrangian approach (CERFACS)

The objective of this task is to propose an alternative to SM and MOM to compute the evolution of the soot particle population by means of a semi-deterministic Lagrangian approach. Contrary to Monte-Carlo stochastic Lagrangian approach, the proposed method computes the trajectories of physical particles. Collisions are treated as stochastic processes. To limit the computational cost, not all physical particles are computed, but only a subset of representative particles that are possibly present in a control volume. This new model has been proposed by CERFACS within the SOPRANO H2020 project and coupled to a simple reduced chemistry (with acetylene as soot precursor). First comparisons with measurements in the ISF3-Target Flame3 configuration have shown the capacity of the model to correctly reproduce the flame structure and soot volume fraction for one operating point. Following the SOPRANO project, **ASTORIA** will allow to improve the method in terms of best trade-off between accuracy, statistical convergence and computational cost. In addition, the model will be extended to take into account the reduced gaseous chemistry including PAH of WP1.1. The resulting model will be evaluated on the 2 other operating points available in the ISF3-Target Flame 3 configuration.

#WP1.3: Generation of soot aggregate morphology (CORIA-CERFACS)
The DLCA code developed by CORIA will be used for the generation of virtual aggregates in order to generate particles with realistic sizes and morphologies. The first step will be the consolidation of the implementation of particle surface growth and oxidation/fragmentation in the "physical" DLCA code. But, in the present case, the research impact of such phenomenon is not in the description of the particles volume fraction but in the formation of realistic morphologies (size distribution of the

primary spheres, fractal dimension, and distribution of the primary sphere overlapping). Recent developments by ETH Zürich have proven the feasibility of such approaches (Kelesidis 2017)
The second step consists in generating such aggregates based on the thermodynamically histories encountered by the particles during their growth in the ethylene-air flames numerically investigated in WP1.1, i.e. a laminar Mc Kenna burner and a swirled turbulent burner. Both will share some extractions of flow parameters (temperature, oxidative and surface growth species concentrations) along PM Lagrangian trajectories from their simulations which will be used by CORIA to generate a statistical set of virtual modelled aggregates representative of the considered flames. In order to validate that approach, the so generated particles morphological characteristics will be compared with detailed results of the literature in the particular case of target flames (McKenna burner for example).

- **WP2: Modelling for radiation of sooting flames in the IR and visible frequency range (RAPSODEE-CERFACS-CORIA)**

Leader: CORIA	Partners: CORIA, RAPSODEE	Start / End: M12/ M36
Main objective	**Modelling PM radiative properties accounting for their morphology**	
Work Programme	**WP 2.1**: Radiative properties of individual aggregates (CORIA) **WP 2.2**: Thermal radiation of sooting flames (IR domain) (RAPSODEE-CERFACS) **WP 2.3**: Computation of a digital image of the flame (visible domain) (RAPSODEE)	
Deliverables	D2.1: Synthesis of the evaluation of the simulated flames individual soot particles (CORIA, M30) D2.2: MCM3D including scattering of soot particles and the RDG-FA code from CORIA (RAPSODEE, M36) D2.3: Simulation of the virtual image by Monte Carlo (RAPSODEE, M36)	

The objective of WP2 is to improve the simulation of radiation both in the infrared and the visible frequency ranges by accounting for soot aggregate morphology when evaluating their radiative properties.

#WP2.1: Radiative properties of individual aggregates (CORIA)
This work package is at the interface between the virtual generation of the aggregates focused on in WP1.2 and the evaluation of the flame radiative properties (WP2.2 and WP2.3). Indeed, the solving of the radiative transfer equation (RTE) necessitates the prior knowledge of the radiative properties of individual aggregates. The simplest approach consists in using the Mie theory but this approach suffers of the hypothesis of spherical particles and has been shown to be not valid for real soot particles (Dobbins et al., 1994). Rayleigh Debye Gans Theory for Fractal Aggregates (RDG-FA) is a simple asymptotic theory that can easily be implemented in RTE solvers. But recent investigations by CORIA and EM2C (Okyay et al. 2014) have shown that realistic morphologies (necking (Yon et al 2015), overlapping (Liu et al. 2016, Donner et al. 2017) can affect the reliability of that theory depending on the considered wavelengths (Yon *et al*, 2014). In consequence, based on the virtual aggregates generated in WP1.2, CORIA will evaluate the particle radiative properties for a range of wavelengths of interest for diagnostics (visible) and thermal radiations (infrared). Absorption and scattering cross sections will be determined by solving the light-particle interaction electromagnetic problem with the use of the DDSCAT code. If possible, these results will be used to evaluate correction factors to be applied to the RDG-FA for integration as simple as possible in the RTE solver (WP2.2). Radiative properties determined for infrared wavelengths will serve as entry for WP2.2 and the obtained in the visible range will be used for WP2.3 in order to enable a direct comparison between simulations and experiments.

#WP2.2: Thermal radiation of sooting flames (IR domain) (RAPSODEE-CERFACS)

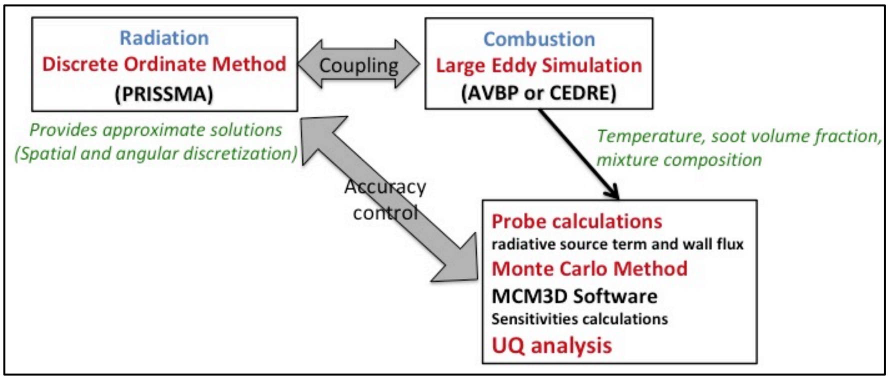


*Figure 4: Approach proposed in **ASTORIA** to accurately model radiative transfer. PRISSMA is a fast radiative solver based on DOM and used for coupling. MCM3D is the reference solution solver*

The objectives of WP2.2 are threefold. i) Implement in PRISSMA the absorption coefficients from WP2.1 and evaluate approximate radiative transfer solutions ; ii) provide reference computations for the radiative transfer using the open source code MCM3D and accounting for the radiation properties provides in WP2.1; iii) assess the uncertainties associated to radiative properties of soot. Both the LII database and the ISF3-Target Flame3 configuration will be studied in this task.
Comparing approximate solutions using PRISSMA and reference solutions using MCM3D has been initiated in the FNRAE project STRASS (2009-2012) and improved in the ANR project SMARTLECT (2012-2016). The whole chain enabling to use as inputs of the two radiation codes a 3D turbulent sooting flame solution from AVBP and to compare radiation results will be re-used in **ASTORIA**. Compared to former projects, MCM3D will need to perform a multiple dimension-integration over the space of multiple-scattering paths. As Monte Carlo is the reference method, here it will include scattering of soot aggregates even if it is negligible in the IR range (Eymet *et al.* 2002*)*. On the other hand, diffusion will be neglected in the PRISSMA solver.
The developments made in the present project will anticipate a significant increase of the LES resolutions for large combustion configuration scales by making use of a recent theoretical proposition, allowing to maintain a strict orthogonality between statistical algorithm and data-representation (Galtier et al. 2013). This essentially means that the question of accessing the data is identified as a separate computer-engineering task: the LES grid will never appear in the radiative transfer part of the algorithm (the optical paths will not be followed across successive meshes). Moreover, these advances have inspired in turn the cutting edge developments in the most demanding graphical industry (Walt Disney animation studio) in order to get a visually representation of clouds (Novak *et al.* 2014) (see *Figure 5*). RAPSODEE is also involved (as an expert) in another project to model cloud radiative effects in atmospheric models (ANR project HighTune, 2016-2020) to obtain an accurate modelling of radiative transfer and provide uncertainties associated to radius distribution of water droplets.

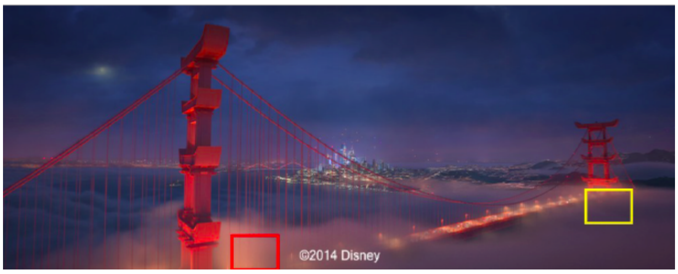


Figure 5: Null collision algorithm from Galtier et al. 2013 applied to the film industry (Walt Disney Animation studios) to get a visually accurate representation of clouds

#WP2.3: Computation of a digital image of the flame (visible domain) (RAPSODEE)
This task aims at improving the numerical method for producing virtual scattering experiments. Today, there are to main approaches to measure soot particle size. Ex-situ sampling methods can be used but require some assumptions and simplifications (interpretation of mobility diameters for example) due to the complex morphology of the soot particles which reduces the accuracy of the measurements. A second approach consists in developing optical techniques based on scattering properties. The main difficulty of this approach is to interpret the signals with the help of simplified theories such as RDG-FA which ignore important phenomena such as multiple scattering inside and between aggregates. In this project, we propose to include these phenomena in the simulations. Thus, it appears that a comparison between the simulations and the experimentally determined planar light scattering signals is the most direct and complete way to validate the ability of CFD-DLCA coupling to simulate the particle sizes.
To achieve this goal, we propose to provide, for the simulated flames in WP1 and WP2, digital images of virtual scattering experiments (scattering or incandescence). A new algorithm needs to be developed in order to simulate a photon path between the laser source and the sensor of the CCD camera. Path tracking is difficult because the sensor is very localized (directional space) and the incoming laser is collimated. As described in WP2.2, this question has already been addressed in meteorology for clouds observation (ANR project High Tune), or film industry (Kutz and al., 2017). The simulated experiments will be compared with results reported in the literature.
The approach developed within WP2.3 will be applied within the **ASTORIA** project to the MICADO test-rig perform in order to compare numerical simulations with light scattering experiments (WP3.3).

- **WP3: Application in a real aeronautical burner (CERFACS-CORIA-ONERA-RAPSO-DEE)**

Leader: ONERA	Partners: All	Start / End: M6 / M48
Main objective	Application of the multiphysics chain to the MICADO kerosene-air test-rig	
Work Programme	**WP 3.1**: Coupled combustion-radiation simulation (CERFACS-RAPSODEE) **WP 3.2**: Soot scattering patterns - **WP 3.2.1:** Experimental campaign of measurement of planar light scattering by soot (CORIA-ONERA) - **WP 3.2.2:** Digital image of the flame (RAPSODEE) **WP 3.3:** Comparison and analysis of the experimental and numerical results (ALL)	
Deliverables	D3.1: Coupled combustion/radiation simulations (CERFACS, M42) D3.2: Report on the experimental campaign of measurement of planar light scattering by soot (CORIA-ONERA, M18) D3.3: Computation of the digital image of the MICADO burner (RAPSODEE, M42) D3.4: Comparison and analysis of experimental and numerical results in the infrared and visible frequency ranges (ALL, M48)	

To demonstrate the feasibility and relevance of the methods developed in WP1 and WP2 in complex geometries, the whole chain including PM production and aggregate formation by combustion, as well as gas and soot thermal radiation and soot visible radiation, will be applied to the MICADO test-rig.

#WP 3.1: Coupled combustion-radiation simulation of soot production (CERFACS-RAPSODEE)
Coupled combustion-radiation simulations will be performed by CERFACS using the AVBP LES solver and the PRISSMA radiation solver. Moreover, RAPSODEE will generate reference solutions for radiation at specific points of the domain selected by all the partners using MCM3D to assess the accuracy of the PRISSMA solver. Whereas the developments for the gas phase chemistry (WP1.1) and the PM particle production (WP1.2) will be used in AVBP, the radiation codes will be improved with

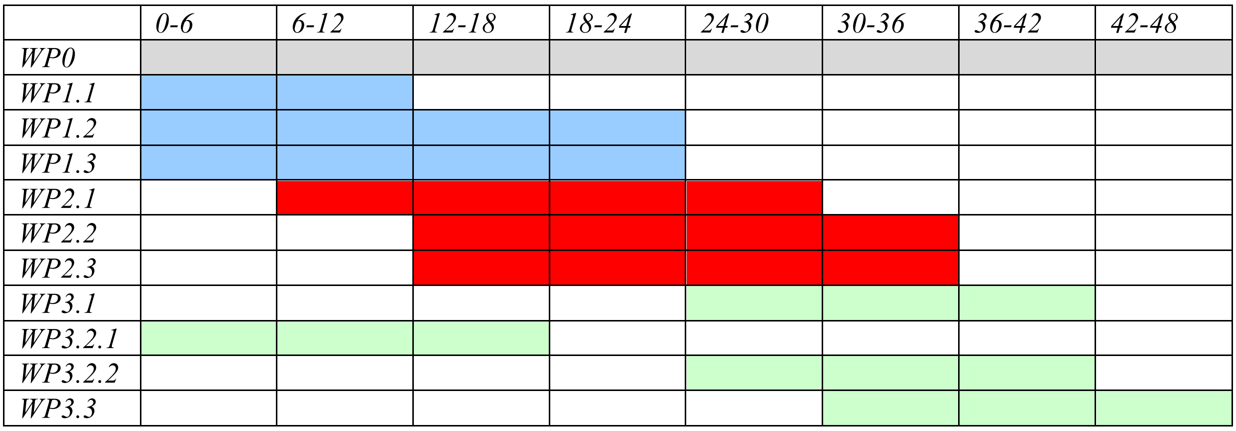
the radiative soot properties depending on their morphology (WP2.1) and the scattering effect (WP2.2).

#WP 3.2: Soot scattering patterns
#WP 3.2.1: Experimental campaign of measurement of planar light scattering by soot (CORIA-ONERA)
CORIA will participate to an experimental campaign of measurement of planar light scattering by soot in the MICADO combustion facility. CORIA will bring a double frequency YAG laser (in order to work at 532 nm) and the intensified cameras for the collection of the signals. The operating conditions considered will be the same as in the SOPRANO project, i.e., pressure levels ranging from 5 to 20 bar, and thus representative of a real combustion chamber. Thus, besides the acquisition of measurements of light scattering due to the presence of soot particles, the SOPRANO data acquired under the same conditions, will be advantageously used (CARS, PIV, soot concentration ...).

#WP 3.2.2: Digital image of the flame (RAPSODEE)
RAPSODEE will apply the algorithm developed in WP2.3 which allows to simulate a photon path between the laser source and the sensor of the CCD camera to compute a digital image of the flame at the same operating points as in WP3.2.1.

#WP 3.3: Comparison and analysis of the experimental and numerical results (ALL)
This task aims at comparing in details the experimental and numerical results in terms of flame structure, soot production and radiation in the infrared and visible frequency ranges. Indeed in addition to the measurement of planar light scattering by soot planned in WP3.2.1, **ASTORIA** will benefit from the huge database generated within the SOPRANO project on the MICADO test-rig to evaluate in details the accuracy of the methodology proposed in **ASTORIA**.

<u>**GANTT CHART**</u>
By construction the Work Packages are scheduled in a chronological order, with overlapping time periods to allow for a good interaction between the different tasks. Only WP3.2 starts early compared to the other tasks of WP3, as it is a separate measurement campaign and is scheduled at the same period as the measurement campaign planned in the SOPRANO project to reduce the costs.



<u>**Scientific and technical justification of requested resources**</u>

CERFACS requests funding for 16 PM of permanent researcher (12 PM for the coordinator and 4 for senior researcher) as well as 24PM for a PhD student to perform numerical work from WP1.2 and WP3.1 (the other 12PM will be supported by CERFACS itself). Travel costs correspond to project meetings, and at least one conference for the PhD student. Computing resources for simulations of combustion will be provided by CERFACS.

CORIA requests funding for the salary of the PhD student and the provision for computing material. The scattering measurement campaign on MICADO bench will require the provision for laser light source, optics and intensified camera as well as the participation of qualified staff. Missions costs will cover the regular project meetings but also some international conferences.

ONERA requests funding for **1)** 6,4 PM [PhD student - permanent personnel] to develop a new soot formation model in strong interaction with CERFACS in WP1.1, **2)** 5,6 PM [engineer - permanent personnel] to carry out the numerical simulation of WP1.1 using CEDRE and perform comparison with the available experimental data, **3)** 5,5 PM [engineer - permanent personnel] to carry out, in collaboration with CORIA, an measurement campaign on MICADO experimental set-up, at different pressure levels in WP3.2, **4)** 3,5 PM [Expert ingeneer - permanent personnel] to ensure the technical coherence of the project and the follow up of the ONERA tasks. Travel costs correspond to progress meetings and at least one conference for the PhD student. Computing and installation costs for simulations and implementation of the high pressure combustion tests will be provided by ONERA.

RAPSODEE requests funding for 6 PM of permanent researcher, and will recruit a postdoc student for one year to perform the numerical work in WP2.2, WP2.3 and WP3.3. The implementation of the different algorithms developed within the project in EDSTAR environment consists in IT engineering tasks and will be performed by a software company (12PM). In this part, there is also a research task at the computer/physics science interface which consists in implementing the null collision algorithm. Moreover a specific data layout has to be designed to use data produced by combustion codes for the Monte Carlo Algorithms. This task has to be led between specialists of radiative transfers and computer graphics researchers. Travel costs correspond to project meetings. Computing resources for radiation simulations will be provided by RAPSODEE.

III. Impact and benefits of the project

The topic and objectives of **ASTORIA**, which aims at reducing PM emissions by combustion system, is fully in line with the objectives of the Challenges "Une énergie propre, sûre et efficace" and "Mobilité et systèmes urbains durables". The direct expected impact of **ASTORIA** can be broken down into several aspects:

- On the fundamental scientific level, **ASTORIA** will allow significant progress on a topic still rarely addressed, namely the soot particle morphology and its impact on the particle evolution and the combustion system through chemistry and radiative properties.
- On the methodological level, a significant result of **ASTORIA** will be an innovative, computationally efficient comprehensive numerical approach to account for all physical phenomena involved in soot formation and emission. It paves the way to original numerical methods and experimental validation approach.
- On a practical application level, **ASTORIA** will bring significant improvement on the prediction of soot emission by combustion in industrial systems and greatly help the design of new environment-friendly combustors. This concerns the transportation sector where clean engines are needed for ground vehicles, planes or helicopters, but also the energy sector running ground-based gas turbines, furnaces or boilers.

ASTORIA will also have long-term, indirect impacts on side topics such as a better evaluation and characterization of anthropic soot emissions in climate models, with an improved description of their radiative forcing. Another generic result of **ASTORIA** will be the improvement of optical diagnostics of soot by integrating more accurate radiative properties. This will allow more direct comparison between simulation and experiment, as will be demonstrated in **ASTORIA** with the concept of "digital image".

All the obtained results (data, reports and codes developed in the framework of the project) will be made available to the scientific community by various means:

- A project web site will propose the publishable reports and data for download.

- The scientific results will be published in high-impact journals in the concerned fields (combustion, fluid mechanics, heat transfer, computational science, experimental techniques). It is expected to publish at least 5 articles during the project.
- The partners will set up a framework and free licence policy for the distribution of the codes developed in **ASTORIA**. For example, the radiation code of RAPSODEE is already open-source; **AVBP** developed by CERFACS can be obtained for free under a licence agreement, and will include the developments of WP1; the **DLCA** code developed by CORIA will be freely distributed after valorization of the results obtained within **ASTORIA**.
- The partners will propose on-line training on the codes developed in **ASTORIA** in view of their application to configurations relevant for soot prediction.

During the last year of the project, a Workshop will be organized on the topic of soot emission by combustion devices. For a high visibility the event will be organized in collaboration with the Groupement Français de Combustion (GFC) and the Société Française de Thermique (SFT). It will be open to the international community, to exchange about recent advances in the field and expose the results of **ASTORIA**.

Particular attention will be put on an efficient exploitation of results. This will require first to specify intellectual property rights (IPR) in the Consortium Agreement, addressing the different cases of data, publications and software. The project results will be advertised in the industrial sector thanks to the privileged relationships of the partners with the aviation and energy sectors (Safran, Airbus, CNES, Renault, TOTAL, EdF, etc.). In particular, the new models developed in **ASTORIA** will be made directly available to CERFACS stakeholders through the code AVBP.

IV. References related to the project

- A. Bescond, J. Yon, F.X. Ouf, D. Ferry, D. Delhaye, D. Gaffié, A. Coppalle, C. Rozé. Automated Determination of Aggregate Primary Particle Size Distribution by TEM Image Analysis: Application to Soot. Aerosol Sci. Tech., 48(8), 2014.

- R. Ceolato, M.J. Berg, N. Riviere. Spectral and annular light-scattering from silica fractal aggregates. J. Quant. Spectrosc. Rad. Trans, 131:160-165, 2013.

- De La Torre and al..”Monte Carlo Advances and concentrated solar applications “, Solar Energy, 103, pp 653-681, 2014

- R.A. Dobbins and C.M. Megaridis. Morphology of flame-generated soot as determined by thermophoretic sampling, Langmuir , 3 (2) :254–259, 1987.

- Dobbins, R. A. and Megaridis, C. M. Absorption and scattering of light by polydisperse aggregates. Appl. Opt. 30:4747-4754, 1991.

- N. Doner, F. Liu, and J. Yon, "Impact of necking and overlapping on radiative properties of coated soot aggregates," Aerosol Science and Technology, vol. 51, pp. 532-542, 2017/04/03 2017.

- B.T. Draine and P.J. Flatau. User guide for the discrete dipole approximation code DDSCAT 7.3. *arXiv preprint arXiv:1305.6497*, 2013.

- C. Eberle, P. Gerlinger, M. Aigner. A sectional PAH model with reversible PAH chemistry for CFD soot simulations. Comb. Flame, 179:63-73, 2017.

- Eymet V., Brasil A.M., El Hafi M., Farias T.L., Coelho P.J., « Numerical Investigation of the effect of Aggregation on the Phase Function and Scattering coefficient of soot in the Infrared region and Radiative Transfer", Journ. of Quant. Spect. and Rad. Trans, 74, 697-718, 2002 .

- Eymet. V., Poitou D., Galtier M., El Hafi M., Eymet V., Fournier R., "Null collision meshless Monte Carlo: Application to the validation of fast radiative transfer solvers embedded in combustion simulators", Journ. of Quant. Spect. and Rad. Trans, vol. 127, 52-59, 2013.

- A. Felden, E. Riber, B. Cuenot. Impact of direct integration of Analytically Reduced Chemistry in LES of a sooting swirled non-premixed combustor. Comb. Flame, 191:270-286, 2017.

- M. Galtier et al. Integral formulation of null collision monte carlo algorithms. J. of Quantitative Spectrosc. and Rad. Trans., 125:57-68, 2013.

- L. Gallen, A. Felden E. Riber, B. Cuenot. agrangian tracking of soot particles in LES of gas turbines. Accepted in Proc. Comb. Inst, 2018.

- K.P. Geigle, M. Köhler, W. O'Loughlin, W. Meier. Investigation of soot formation in pressurized swirl flames by laser measurements of temperature, flame structures and soot concentrations. In Proc. Comb. Inst., 35(3):3373-3380, 2015.

- L. Y. M. Gicquel and G. Staffelbach and T. Poinsot. Large Eddy Simulations of gaseous flames in gas turbine combustion chambers. Prog. Energy Comb. Sci., 38(6):782-817, 2012.

- N. Gourdain, L. Gicquel, G. Staffelbach, O. Vermorel, F. Duchaine, J.-F. Boussuge, et al., High performance parallel computing of flows in complex geometries - part 2: applications, Comput. Sci. Disc, 2 (2009) 28pp.

- P. Jourdaine, C. Mirat, J. Caudal, A. Lo, T. Schuller. A comparison between the stabilization of premixed swirling CO_2-diluted methane oxy-flames and methane/air flames, Fuel, 201(1), 2017.

- P. Kutz, R. Habel, Y.K. Li and J. Novak. ACM Transactions on Graphics (TOG), 2017.

- M.E. Mueller, H. Pitsch. LES of soot evolution in an aircraft combustor. Phys. Fluids, 25(11), 2013

- J. Novak, A. Selle, W. Jarosz. Residual ratio tracking for estimating attenuation in participating media. ACM Transactions on Graphics (TOG) (Proc. of SIGGRAPH), 33(6):179, 2014.

- G. Okyay and F. Enguehard. Effect of fractal parameters of soot aggreagates on their absorption and scattering properties simulated by discrete dipole approximation. In *10th Int. Conf. Series on Laser-light and Interact. with Particles*, Aug 2014, Marseille, France.

- P. Rodrigues, B Franzelli, R Vicquelin, O Gicquel, N Darabiha. Unsteady dynamics of PAH and soot particles in laminar counterflow diffsion flames. In *Proc. Comb. Inst.* 36 (1) :927-934, 2017.

- C. Saggese, S. Ferrario, J. Camacho, A. Cuoci, A. Frassoldatti, E. Ranzi, H. Wang, T. Faravelli. Kinetic modeling of particle size distribution of soot in a premixed burner-stabilized stagnation ethylene flame. Comb. Flame, 162(9):3356-3369, 2015.

- J. Yon, F. Liu, A. Bescond, C. Caumont-Prim, C. Rozé, F.X. Ouf, A. Coppalle. Effects of multiple scattering on radiative properties of soot fractal aggregates. J. . Quant. Spectrosc. Rad. Trans, 133:374-381, 2014.

- J. Yon, A. Bescond, and F. Liu, "On the radiative properties of soot aggregates part 1: Necking and overlapping," Journal of Quantitative Spectroscopy and Radiative Transfer, vol. 162, pp. 197-206, 2015.

Requested means by item of expenditure and by partner*

<table>
<tr><th colspan="2"></th><th>Partner CERFACS</th><th>Partner CORIA</th><th>Partner ONERA</th><th>Partner RAPSODEE</th></tr>
<tr><td colspan="2">Staff expenses</td><td>120 000 € (non permanent) + 64 000 € (permanent)</td><td>99 500 € (non perm.) + 59 149 € (permanent)</td><td>164 915 €</td><td>60 586 € (non permanent) + 38 448,50 € (permanent)</td></tr>
<tr><td colspan="2">Instruments and material costs (including the scientific consumables)</td><td></td><td>27 000 €</td><td></td><td>5 000 €</td></tr>
<tr><td colspan="2">Building and ground costs</td><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="2">Outsourcing / subcontracting</td><td></td><td></td><td></td><td>50 000 €</td></tr>
<tr><td rowspan="2">General and administrative costs & other operating expenses</td><td>Travel costs</td><td>10 000€</td><td>15 000 €</td><td>5 000 €</td><td>5 000 €</td></tr>
<tr><td>Administra-tive manage-ment & structure costs**</td><td></td><td></td><td></td><td></td></tr>
<tr><td colspan="2">Sub-total requested</td><td>120 550 €</td><td>152 820 €</td><td>141 203, 60 €</td><td>130 232,88 €</td></tr>
<tr><td colspan="2">Requested</td><td colspan="4">544 806,48 €</td></tr>
</table>

* The amounts indicated here must be strictly identical to those entered on the website. If both information are not consistent, if they were badly filled in or lacking, the information entered online will prevail on those reported in the submission form / scientific document.
** For marginal cost beneficiaries (mostly public partners), these costs will be a package of 8% of the eligible expenses. For full cost beneficiaries (mostly private partners), these costs will be a sum of max. 68% of staff expenses and max. 7% of other expenses.