PHD SUBJECT FOR SEPTEMBER 2019

Title : Modelling the radiative properties of soot fractal aggregates with realistic morphologies.

Scientific Domain: Optical diagnostic / soot radiative properties.

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Related program: ANR ASTORIA

Abstract:

In the context of the ANR project "ASTORIA", the CORIA laboratory aims to enhance the virtual conception of soot particles during their transport and formation in flames, in particular in terms of morphology and radiative properties. The numerical aspect of this work consists in establishing a database of soot particles radiative properties computed with the Discrete Dipole Approximation method. That database will be used to improve the Rayleigh Debye-Gans Theory for Fractal Aggregates (RDG-FA) by proposing some correction factors depending on the morphological and optical properties of realistic soot particles. The experimental part consists in applying some laser-based optical diagnostics in target flames in order to quantify the concentration, size distribution and morphology of the particles and to compare with the results of the CFD modelling done by a partner laboratory.

Description of the subject:

The increasing energy demand, hazardous effects on human health produced by combustion generated ultrafine particulate emissions and unprecedented concerns of emissions from combustion systems on global warming and climate change have led to increasingly stricter regulations on exhaust emissions from combustion devices, especially in the context of aeronautical sources. The current estimate puts soot particles as the second largest contributor to climate change, just after carbon dioxide (CO2). Unlike CO2, soot particles have a fairly short life span in the atmosphere, on the order of few weeks. Consequently, it has been suggested that a reduction of soot emissions from combustion systems and vehicles is an effective means to slow down global warming and climate change. On the other hand, soot particles formed in practical combustion system are important mainly because their significant contribution to radiant heat transfer and thus their presence is desirable in some systems, such as boilers and furnaces.

CFD is becoming a useful tool for the design and conception of engines. Nevertheless, soot modelling remains a hard task due to the complex mechanisms involved in soot formation. In particular, the current modelling of soot in CFD codes (sectional codes, moment methods, semi empirical models, etc.) is morphologically simplistic since equivalent spheres are considered. Unfortunately, it was shown that equivalent sphere approximation (use of the Mie theory) leads to huge errors in what concerns the evaluation of soot radiative properties [1]. In parallel, the virtual conception of realistically soot particles' morphologies is generally ensured by the use of Diffusion Limited Cluster Aggregation (DLCA) codes that generally suffer, in counterpart, of a lack of physics for the particles generation (monodisperse primary sphere, no residence time, no surface growth…).

To solve those limitations, a strategy of coupling CFD and DLCA codes is under evaluation in the context of the ANR project ASTORIA. Schematically, that project can be divided in two parts. The first one consists in generating virtual realistic soot particles by coupling results from CERFACS's AVBP code and CORIA's DLCA code. Different target burners will be considered, from simple academic flames to more complex burners representative of aeronautical applications. This part of the project is ensured by a PhD work, which has already started. The second part of the project will be ensured by the current PhD recruitment. It consists in determining the individual particles radiative properties (absorption, scattering cross sections) by solving the Maxwell equations on the realistically soot particles generated in part one of the project. The resolution will be ensured by using DDSCAT [2] code by exploiting the numerical resources of CRIANN. **The main objective of the current work is to provide a useful and physically discussed corrections factors to bring to a simple analytical theory of light interaction with fractal aggregates** (Rayleigh Debye Gans-Theory for Fractal Aggregates : RDG-FA [3]) based on the analysis of the so obtained database [4-8]. Indeed, RDG-FA theory can be integrated in Monte-Carlo solvers for the Radiative Transfer Equation (ensured by the Rapsody laboratory in the ASTORIA project). This will ensure the determination of the thermal radiation by the simulated flames as well as "virtual experiments" based on the simulation of optical diagnostic experiment (planar laser light scattering) that will be compared to real experiment on similar setups. This represents a very innovative way to validate soot modelling in CFD codes. In order to compare the simulations with the experiment, in addition to the numerical evaluation of the radiative properties of soot particles, **the recruited PhD will also experimentally characterize the soot particles produced in configurations identical to modeled flames**. The measured quantities like soot production, geometric mean diameter of soot particles, polydispersity, overlapping, fractal dimension, (etc…) will be established or derived directly from Line of Sight Attenuation (LOSA), angular or spectrally resolved light scattering, Laser Induced Incandescence (LII) technique [9] or Transmission Electron Microscopy analysis [10, 11].

PhD program (36 months):
Months 1-6 Bibliography
Months 7-12 learning DDSCAT, LII and light scattering techniques through some test cases.
Months 13-21 Experimental characterization of the target flames selected in the project. Determination of the corresponding soot optical index. A campaign of measurement is also planned on the Mikado test rig at Onera.

Months 21-27 Realization of the soot radiative properties database based on CERFACS and CORIA modelling of soot generation.
Months 27-30 Analysis of the database, elaboration of an enhanced RDG-FA.
Months 31-36 Writing of papers and of the manuscript.

Necessary resources :

Computations will be carried out at CRIANN. The experimental setup for optical diagnostic is available and has to be adapted on the selected target burners.

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