CFD and aerosol dynamics Box-MODEL to improve dispersion models

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Introduction

To cope with the environmental requirements and the continuous rise of the air traffic, meeting the air quality objectives is becoming a high constraint for the development of the air transport sector. The long-term objective is to answer to the main concern expressed by the ICAO on air pollution issues generated by the air transport sector on the local air quality in the airport area. The EU Horizon2020 project AVIATOR (2019 – 2022, see aviatorproject.eu) is adopting a multi-level measurement, modelling and assessment approach to develop an improved description and quantification of the relevant aircraft engine emissions, and their impact on air quality under different climatic conditions, specifically on non-volatile PM and volatile PM (down to <10 nm), and volatile PM gaseous precursors. In this framework, the program proposed here is aimed at developing an innovative methodology and tools to increase the capability of prediction for the standard dispersion modelling tools in order to better take into account pollutant sources at micro-scales.

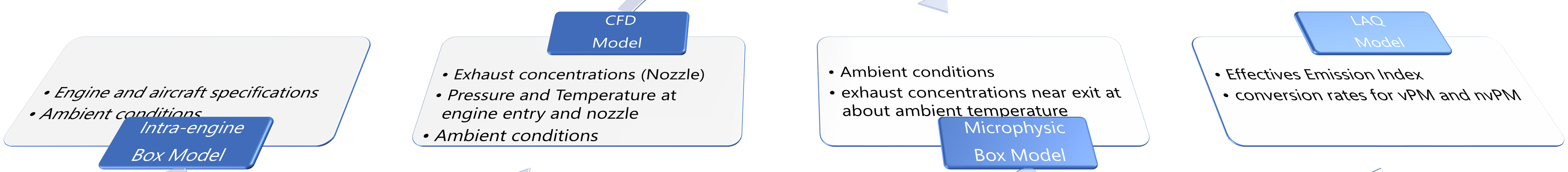
Aims and objectives

One of the project aims is to provide advancing aircraft plume and airport modelling. To reach those objectives, it is necessary:

- to investigate the microphysics and chemistry of pollutant formation and evolution (with emphasis on total PM) from the exit of the main engine and APU to identify limitations of the currently adopted regulatory approach towards an improved representation and parameterisations suitable for use in future dispersion modelling and regulatory standard setting;
- to describe the physical dynamics of the main engine and APU exhaust plume to move towards the development of validated parameterisations suitable for future dispersion modelling and regulatory standard setting. This will specifically consider the interaction of wing tip vortices during take-off and approach.

Methodology: Cascade model

In order to develop an innovative methodology and tools, an original strategy of a so-called cascade model is adopted here. Each model feeds each other to **advance our understanding of microphysical, chemical processes and plumes/vortex interaction** towards an **improved representation** and parameterizations of relevant processes at airport level involving aerosol dynamics. Resutls should provide suitable input for LAQ dispersion modelling, in particular: EIs, conversion rates regarding nvPM and vPM.

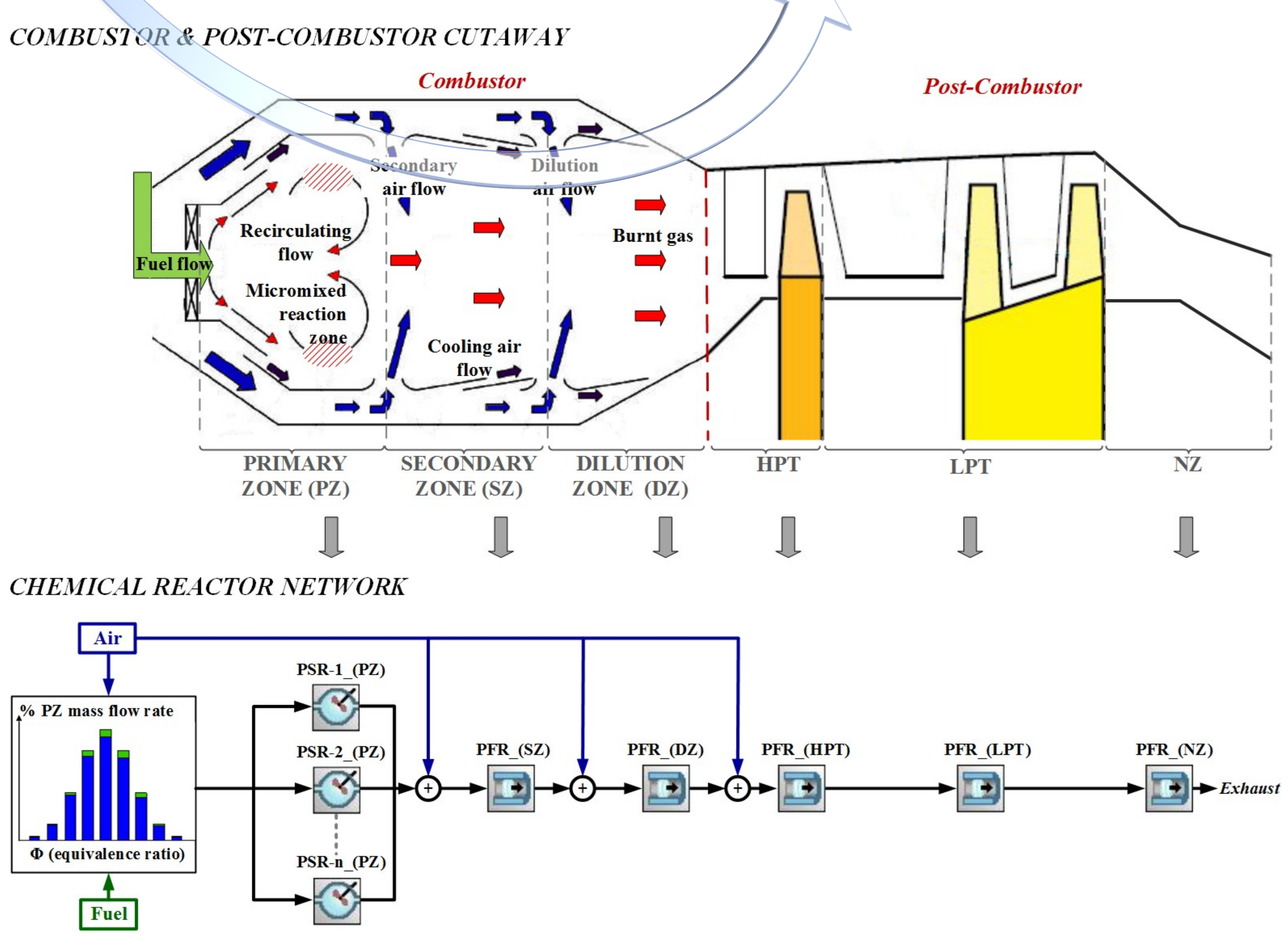


AEROGAS3P[1]: Intra-engine box model (Combustor and Post-Combustor modelling)

A 0-D/1-D gas-turbine model, taking into account combustor, turbine, and nozzles, at different operating conditions, with a Kerosene Jet A1 - kinetics scheme including a soot-kinetics model will be used.

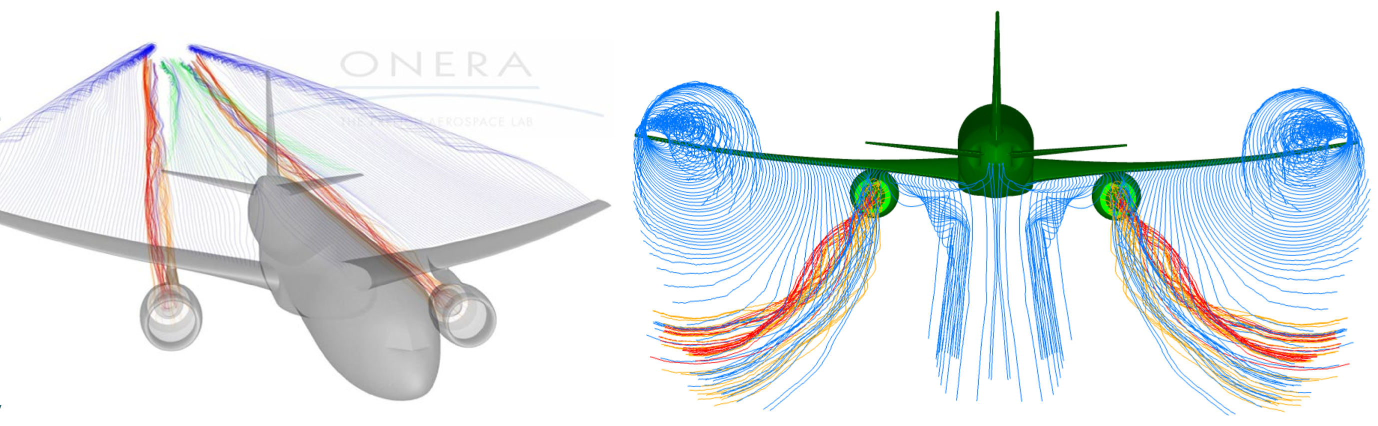
Since jet fuels like Jet A1 are made of several species, a surrogate three-component jet fuel was used. The surrogate is a mixture of n-decane, propylbenzene, and propylcyclohexane. The kinetics included a polycyclic-aromatic-hydrocarbon (PAH) formation and growth mechanism up to benzopyrene molecules (20 carbon atoms and five aromatic rings), allowing the production of soot precursors [1].

This box model is based on a multi-zone representation of combustor in which the reactive flow can be approximated by a 0D/1D behavior. These zones are modeled with simple chemical reactors and are linked together to built a Chemical Reactors Network (CRN). This rather simplified method reduces the level of complexity of a CFD calculation and is very efficient computationally and may be clearly satisfying for parametric studies as needed in air quality modeling. The combustor CRN is constituted of three main zones defined as the primary zone (PZ), the secondary zone (SZ), and the dilution zone (DZ). For downstream secondary and dilution zones in the combustor, flow properties mainly follow a 1-D evolution, and each zone is modeled with a single PFR (Plug Flow Reactor), named PFR_(SZ) and PFR_(DZ). Similarly, to model the evolution of combustion products in post-combustor modules, a CRN of three PFRs in series corresponding to high-pressure-turbine (HPT), low-pressure-turbine (LPT), and nozzle (NZ) modules has been developed.



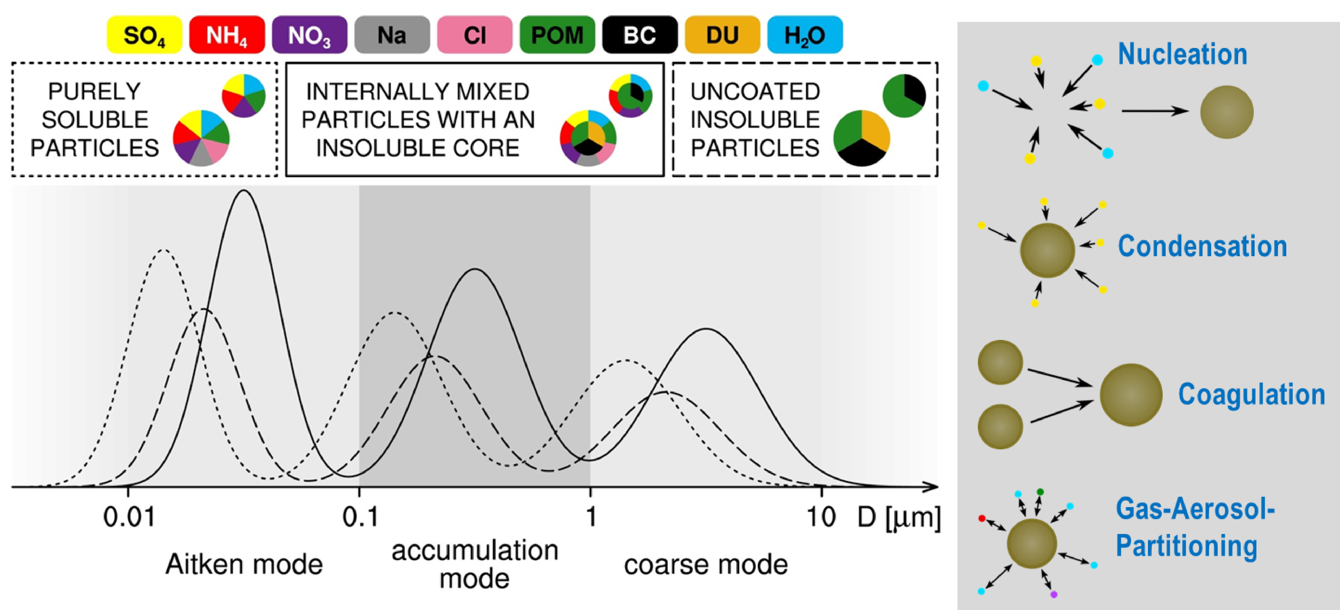
CEDRE[2]: CFD model

ONERA has developed a long term expertise in the field of combustion, engine emission, plume physics and chemistry, contrail formation using various numerical tools, adapted to this physics that has to be addressed. The CEDRE CFD code is then an efficient tool that can be used with the aim of designing installations for example or to model the aircraft and its exhaust properties. It is a parallel, three-dimensional, multi-species, compressible Navier–Stokes solver. The numerical method is based on a cell-centered finite-volume approach for general unstructured grids, especially appropriate when complex geometries such as aircraft, jet engine or installations are used. Combustion models and soot models are available. Gas-phase chemistry can also be implemented in specifying kinetic reaction schemes (for example, including SOx, NOx and HOx chemistry). CFD allows to explicitly model the interaction of the moving aircraft frame and of the emitted exhaust with the ambient flow field but also give plume details such as temperature, pressure, velocity and gas-phase chemistry.



MADE3[3]: Aerosol Box Model

MADE3 aerosol model is capable of describing the concentration, size distribution, composition, and mixing state of particulate matter from aircraft emissions and other sources and simulates aerosol dynamics comprising gas-particle partitioning, gas to particle conversion of low-volatility species, mass transfer between particles by coagulation. For application in the AVIATOR project, the model will be applied as a two-box approach to represent aircraft exhaust as well as the background. The exhaust dilution will be simulated by means of controlled mass transfer from the background into the polluted box. The model will be constrained by initial and boundary conditions according to the results of AVIATOR's exhaust modelling and measurement activities. In addition, simulations from large-scale atmospheric aerosol modelling will be utilized to constrain the large-scale background.



Perspectives

A series of sensitivity studies will be performed comprising aerosol dynamics modelling with MADE3 and systematically evaluated with observations. AVIATOR will utilize the MADE3 results to assess the impact of aircraft emissions on UFP concentrations in and around airports. Moreover, CFD CEDRE simulations improved by the AEROGAS3P intra-engine box model will be used to provide high fidelity data. Comparisons with experimental activities within the AVIATOR project (testbed and on-wing experiments measurements) will be performed. According to the cascade model, those results will be used to upgrade classical dispersion modelling such as LASPORT.

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