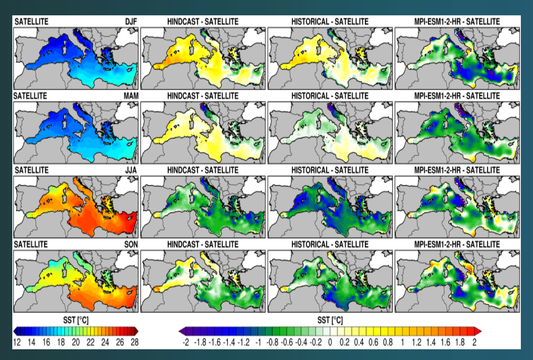
Italian National Agency for New Technologies, Energy and Sustainable Economic Development

CRESCO HPC Applications

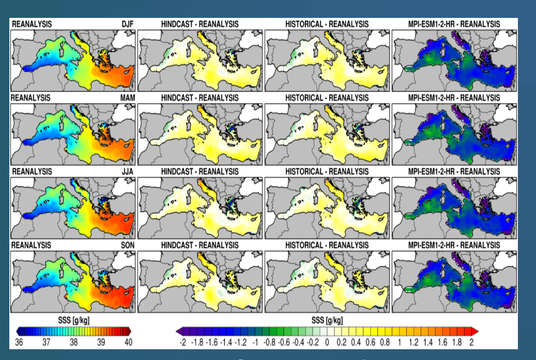
Energy Technologies Department – ICT Division

Environments: Climate Changes

In the framework of the coordinated regional modeling initiative Med-CORDEX (Coordinated Regional Climate Downscaling Experiment), ENEA provides an updated version of the regional Earth System Model ENEA-REG designed to downscale, over the Mediterranean basin, the models used in the Coupled Model Intercomparison Project (CMIP6). The regional ESM includes coupled atmosphere (WRF), ocean (MITgcm), land (Noah-MP, embedded within WRF), and river (HD) components with spatial resolution of 12 km for the atmosphere, 1/12° for the ocean and 0.5° for the river rooting model. For the present climate, ENEA performed a hindcast (i.e. reanalysis-driven) and a historical simulation (GCM-driven) over the 1980-2014 temporal period. The evaluation shows that the regional ESM reliably reproduces the mean state, spatial and temporal variability of the relevant atmospheric and ocean variables.



Sea Surface Temperature



Sea Surface Salinity

Comparison of seasonal sea surface temperature and salinity from satellite data, the ENEA-REG hindcast and historical experiments and the MPI-ESM1-2-HR model. Seasonal averages are computed in the temporal period 1982–2014.

Energy Technologies: Combustion

Mild combustion is one of the promising techniques to reduce pollutant emissions, such as NOx , in combustion processes. It is also a promising technique to burn hydrogen: the highly diluted conditions mitigate its reactivity and its calorific power. The cyclonic flow configuration adopted in this work may represent a proper way to enhance the mixing process while allowing for residence times long enough to achieve complete oxidation of diluted and preheated mixtures. In this work, Large Eddy Simulation (LES) of a Hydrogen/Air cyclonic burner operating in the MILD combustion regime at atmospheric pressure is per- formed using ENEA's in-house code, HeaRT. Accurate molecular transport properties and a reduced chemical mechanism are considered. Radiative and wall heat exchange effects are also modelled. Results show that temperature is quite uniform along the whole burner with an average value of 1350 K, lower than that typically measured in standard hydrogen combustion. This condition leads to a very low NOx emissions, the thermal path being the main NO formation mechanism. The NOx values obtained at the burner outlet are lower than 30 ppm, confirming the possibility of burning hydrogen under MILD combustion conditions.

The test case consists of a prismatic 20x20x5 cm^3 burner (in the x-y-z direction respectively) at atmospheric pressure. Two anti-symmetric couple of jets and the gas exit positioned at the central part of the burner top induce the cyclonic flow-field within the combustor chamber. Each couple of jets is composed of two cylindrical ducts, the oxidizer with an internal diameter of 0.8 cm, the fuel with 0.15 cm. The oxidizer flows are preheated to the inlet temperature of 550 K and injected at 28.9 m/s, while the fuel is 300 K with a velocity of 207 m/s. The walls are set at 1253 K as in the experimental test. The oxidant injectors are located at 2 cm from the lateral walls, whereas the fuel injectors are at 4.5 cm. The domain is discretized through 330x111x250 points in the x,y and z directions respectively. Appropriate refinement of the grid is performed in the regions with higher gradients: the minimum grid width is located near the injection zones with Δx = 85μm, Δy = 130μm and Δz = 350μm.

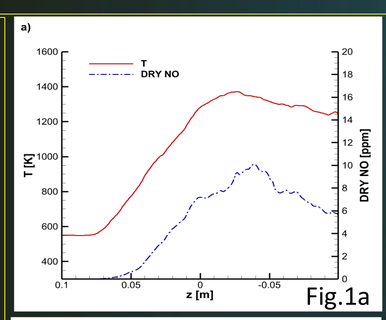


Fig.1a

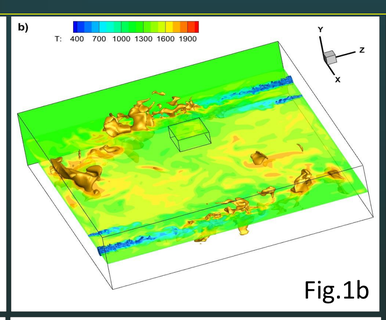
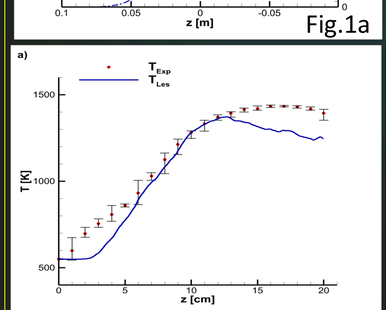


Fig.1b



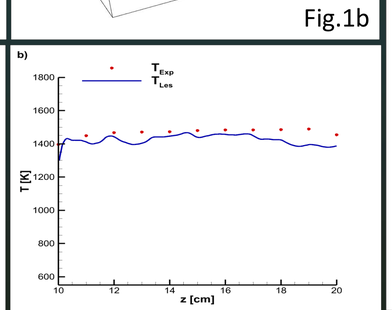


Fig.3

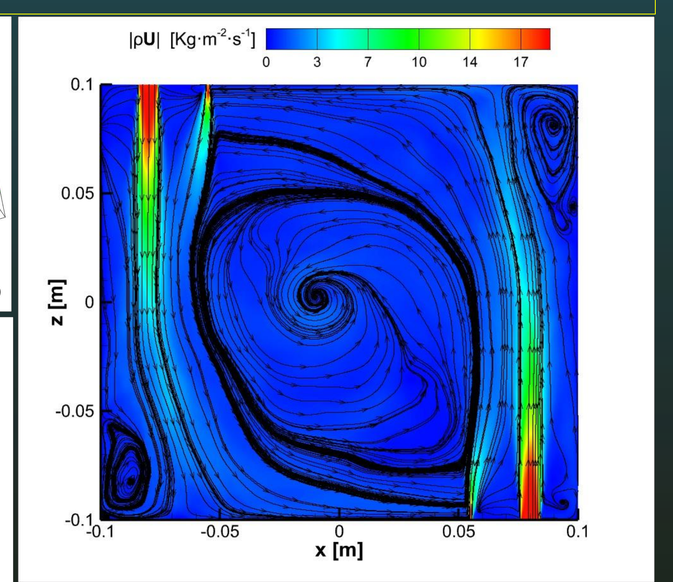
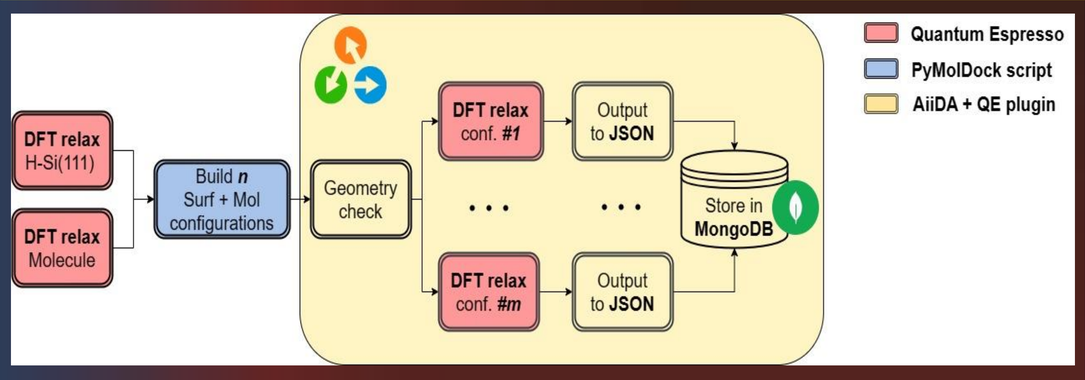


Fig.2

The temperature and NO concentration are sampled with a frequency of 50 kHz on the yz-plane at x = 8 cm. Figure 1a reports the predicted average temperature and the average NO concentration profiles along the air jet axis. The temperature profile is quite uniform from 10 cm downstream of the air injector, with an average value of 1250 K, lower than that typically measured in standard hydrogen combustion. This condition leads to very low NO emissions, the thermal path being the main NO formation mechanism. Figure 1b shows the instantaneous temperature field on a slice at y = 0.025m. Figure 2 shows the average momentum field and the streamlines on a slice at y=0.025m. The trend of temperature obtained with LES is similar to the experimental one, as shown in Fig. 3, and at the reactor center it is consistent with the experimental results, but the error is not negligible at the air jet inlet. The simulation was performed by means of the in-house parallel code HeaRT [7] and ENEA's super- computing facility CRESCO [8](Computational Center for Complex Systems) requiring 3000 CPU hours on 3900 processors. The solution was advanced at a constant time step of 5.9 ns, with a CFL (Courant– Friedrichs–Lewy) set to 0.11, in order to ensure the stability of the numerical methods

Materials Science: Automated Interactive Infrastructure DAtabase (AiiDA)

An automated ab initio calculation workflow has been devised and executed for systematically exploring many potential functional organic molecules along with their corresponding structural configurations for adsorption onto Si surfaces. The objective of this workflow is to assess the stability of various functional groups, enabling the identification of promising candidates for further investigation. The computational power of the ENEA's CRESCO cluster was harnessed to accurately simulate and explore numerous configurations using this workflow. The calculation results are automatically collected and recorded in the database installed on CRESCO.



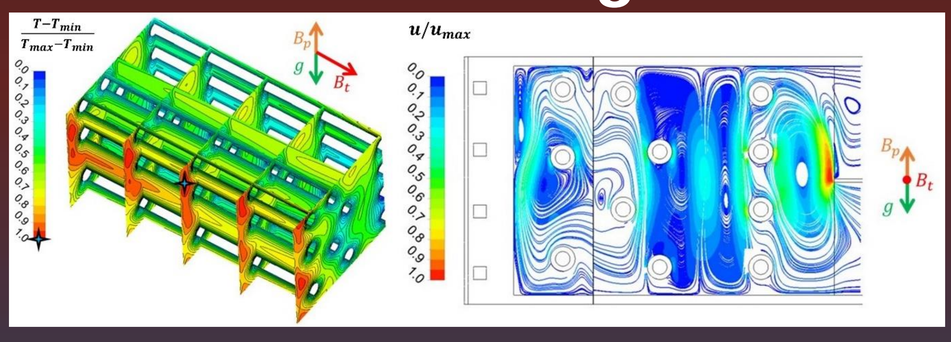
Schematic of the numerical workflow in AiiDA

The steps of workflow have been defined with particular attention to efficiently manage calculation resources, discard redundant configurations, and store the results in a structured manner for further analysis and retrieval. A Builder (PyMolDock) fetches structures files of the organic molecule and the passivated H:Si(111) surface from cloud databases; than two structural DFT relax calculations are performed both for isolated molecule and isolated H:Si(111) slab using Quantum Espresso package; finally the outputs of relaxation calculations are parsed and n distinct structural input files with the molecule grafted onto the surface are generated. The compute tasks are carried out by Quantum Expresso. The workflow above described has been implemented using the AiiDA, incorporating the PyMolDock Python script ENEA have developed and the QE plugin code for carrying out DFT calculations.

Nuclear Fusion: MHD model of Liquid Metal Water-cooled Breeding Blankets

A magnetohydrodynamic analyses is performed to characterize the flow in water-cooled liquid metal breeding blankets are reported. Two cases are considered, both featuring a large number of internal cylindrical obstacles: fully developed forced convection vertical flow with obstacles aligned with the main flow direction and horizontal natural convection with uneven volumetric heating and transverse cooling pipes.

The Breeding Blanket (BB) is a critical component of a fusion reactor which has the fundamental tasks of breed the tritium required for the reactor operations and of extract the thermal power generated by the fusion reactions. The most promising concepts involve the use of a Liquid Metal (LM) as working fluid, the lead-lithium eutectic alloy (PbLi), due to its excellent thermal properties and the possibility to double the coolant role as tritium breeder.



The figure shows the velocity and temperature distribution at Hartmann number H_a = 9159. No temperature fluctuations have been identified after a 100-300s of transient and heat transfer is dominated by diffusive processes with pipe Nusselt numbers ranging from 1.1 to 1.2.