PhD and PostDocs positions - ERC Starting Grant project VADEMECOM

VADEMECOM is an ERC Starting Grant, starting on April 1st 2017, for a duration of 5 years.

VADEMECOM is based on the observation that combustion science will play a major role in the future quest for sustainable, secure and environmentally friendly energy sources. Two thirds of the world energy supply rely on combustion of fossil and alternative fuels, and all scenarios forecast an increasing absolute energy supply through combustion, with an increasing share of renewables. Thus, combustion will remain the major actor in transportation and power generation as well as in manufacturing processes, like steel and glass.

Nevertheless, combustion science will need profound innovation to meet future energy challenges, such as energy efficiency and fuel flexibility, and ensure future generations with affordable and sustainable energy and healthy environment. In this context, MILD combustion represents a very attractive solution for its fuel flexibility and capability to deliver very high combustion efficiency with virtually zero pollutant emissions. Such a combustion regime is the result of a very strong interaction between turbulent mixing and chemical kinetics. The fundamental mechanism of this interaction is not fully understood, thus justifying the need for experimental and numerical investigations.

The overall objective of VADEMECOM is to drive the development of modern and efficient combustion technologies, by means of experimental, theoretical, and numerical simulation approaches. New-generation simulation tools for MILD combustion will be developed, to reduce the dependence on sub-grid models and increase the fidelity of numerical simulations. High-fidelity experimental data will be collected on quasi-industrial systems, to disclose the nature of the interactions between fluid dynamics, chemistry and pollutant formation processes in MILD combustion. Experiment and numerical simulations will be tied together by Validation and Uncertainty Quantification techniques, to allow the ground-breaking application of the developed approaches and promote innovation in the energy sector.

We seek candidates (PhD and PostDoc) with a strong background in the following fields:

1. **Chemical kinetics**. Expertise in reduction methods for chemical kinetics is required. Experience in methodologies for sensitivity analysis, validation and uncertainty quantification of kinetic mechanisms constitutes an asset;
2. **Turbulence chemistry interactions & combustion modelling**. Expertise in Large Eddy Simulation is required. Experience in model reduction represents an asset.

Two positions are readily available in the framework of the project. They are open to both researchers at the PhD (4 years contract) and PostDoc (3 years contract) level. The choice will be based on the candidates' profiles. The open topics are the following:

1. **Homogeneous chemical kinetics for MILD and oxy-MILD combustion**
   The primary purpose of the study is that of revisiting existing chemistry sub-models in the perspective of the non-conventional combustion regimes investigated in the project, i.e.

MILD combustion. In particular, the optimisation of kinetic mechanisms for various energy carriers (natural gas, biogas, syngas and hydrogen/ammonia-enriched fuels) will be carried out using tools such as local and global sensitivity analysis.
The effect of mechanism reduction on prediction uncertainty will be also assessed. The investigation will rely on open source software, DAKOTA and OpenSMOKE++. DAKOTA (dakota.sandia.gov) is a collection of open and customizable algorithms for sensitivity analysis, optimization and uncertainty quantification, available from Sandia National laboratories. It will be coupled to the OpenSMOKE++ suite, a collection of open and customizable solvers for detailed chemistry investigation in canonical reactors, available from Politecnico di Milano, to assess the uncertainty in detailed and reduced mechanisms and generate optimal kinetic models.

2. **Turbulent combustion modelling for the simulations of MILD and oxy-MILD combustion**
The objective of the study will be the development of novel approaches for turbulence/chemistry interactions in MILD and oxy-MILD combustion, using a model-reduction approach developed by the PI research group, that exploits Principal Component Analysis (PCA) to determine the most important variables controlling the behaviour of a chemically reacting system. The model will be initially validated in the framework of high-fidelity simulation tools such as DNS and later extended to LES, assessing the need for sub-grid models (i.e. potential for Implicit LES) and the impact of several sub-grid models (i.e. based on canonical reactors such as PSR and PaSR) on the results.

Offer Requirements

- A MSc or a PhD degree in Engineering, Chemistry, Physics and Applied Mathematics, with a focus on either chemical kinetics, or fluid mechanics and combustion modelling.
- A qualification equivalent to first-class honors degree is preferred.
- Experience in numerical methods, excellent computational skills, experience with C++ programming, interest in CFD programming and turbulent combustion modelling.
- English language is mandatory.

Selection process

The selection process is based on two steps:

- Evaluation of the documents provided by the Applicant
- Interview of each candidate having the eligibility requisites (evaluated through the first step). The interviews will be organized remotely via Skype.

List of Documents to be provided:

- Letter of motivation (approx. 1 page)
- Copies of degree and academic transcripts (with grades and rankings)
- Summary of Master's thesis (approx. 1 page)

- Short CV including a publication list (if any)
- Two reference letters from academics. Candidates must indicate the academics details when applying.
- Proof of English language skills
- Passport copy

Please follow the links for applications and further details.

https://euraxess.ec.europa.eu/jobs/170710