Ph.D. thesis position
Energy and chemical engineering thermodynamics

General information

Topic: Energy and chemical engineering thermodynamics

Title: **Design of reactive working fluids for power cycles.**

Funding: French ministry of Higher Education and Research with the support of the company *Air Liquide*; Possibility to supplement the salary by teaching (only for people speaking French).

Basic salary: 1450 € / month (**after taxes**). 1600 €/month with teaching activities

Dates: September 2021 – August 2024.

Place: Team ThermE (Thermodynamics and Energy) of the LRGP (Laboratory for Reactions and Chemical Engineering) – University of Lorraine, Nancy, France.

Ph.D. supervisors:

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Pre-requisites of the candidate

- Excellent knowledge in mathematics.
- Very good knowledge in thermodynamics and energy engineering. Excellent knowledge of thermodynamic cycles.
- Good knowledge of a computer-programming language (Fortran, Matlab, …).
- Very good communication skills (in English).
- Very good analytical skills.

Application

To apply, send your CV, university grades, and a motivation letter (in English or in French) to both Jean-Noël Jaubert and Silvia Lasala.

Deadline for submission of the application: **30 May 2021.**

■ Scientific content

Keywords: Thermodynamic cycles, Reactive fluids, Thermodynamic and reaction equilibrium calculations, Reaction design, Test rig design, Experimental validation.

■ Introduction

At present, the thermal engine remains the most reliable commercialized technology enabling the conversion of thermal energy into electricity. Although classical thermal engines are particularly suitable for high-temperature and high-power fossil fuelled thermal sources, their employment to convert the lower-grade energy content of renewable and waste heat sources reveals strong performance limitations. As a consequence, the current exploitation of such thermal energy sources, central to the achievement of a sustainable energy system, results to be severely constrained.

This thesis intends to contribute to the development of a highly efficient and extremely compact closed power cycle owing its promising -and still unexploited- performances to the **use of a properly selected equilibrated reactive working fluid, instead of a classical inert one**. Preliminary calculations (see https://doi.org/10.1016/j.enconman.2020.113685) have indeed shown that the simultaneous conversion of the thermal and chemical energy of reactive fluids may result in the extreme intensification of closed power cycles.

■ Objectives and methodology

In this thesis, **the candidate:**

- **will develop an original methodology enabling the selection of existing suitable reactive fluids for different applications of the power cycle** (that is, different thermal sources).

  The approach that will be followed is twofold. The research of the reactive fluid will be performed, on the one side, considering reactions whose thermodynamic and kinetic data are present in available databases and, on the other, designing reactions with specific enthalpy, entropy of reaction and kinetics. A pivotal tool to be developed to design new reactions with specific kinetics is a predictive kinetics calculation code relying on Quantum Chemistry calculations.

- **will develop a test rig enabling the validation of the theoretical calculations performed in the first part of the thesis.**

  This experimental apparatus will consist in a micro-power cycle initially tested with pure gaseous CO_2 and, in a second time, with a preliminary selected reactive fluid. A micro-turbine of 5 kW_{el} has already been bought, while the rest of the experimental test rig will be acquired and installed during – and thanks to – the development of the thesis. Experimental measurements of the reactive fluid composition all along the cycle will be performed by online Raman spectroscopy measurements.