Internship offer for Master 2 or last year engineer student

CFD simulation of the volatilization of the metal alloy oxide layer exposed to oxidizing and humid environments at high temperatures

Every year, corrosion is responsible worldwide for significant additional costs to ensure the reliability of metal structures. Moreover, the industry must face many challenges, such as increasing process yields to reduce greenhouse gas emissions or the implementation of greener energies, which often imply more severe conditions of use for metal parts, in particular in the presence of water vapor, and thus an increased risk of corrosion.

To ensure their good durability against corrosive environments at high temperatures, metal alloys must form on the surface a protective oxide layer, that is to say stable, adherent, dense and slow growing. Alumina Al_2O_3 and chromine Cr_2O_3 meet these criteria. However, beyond 600 °C, two phenomena are observed in the case of chromino-forming alloys subjected to oxidizing and water vapor-rich atmospheres. On the one hand, the formation of chromine by reaction between oxygen and the alloy ensures the protection of the alloy. On the other hand, the reaction between chromine and the oxidizing and humid environment produces a volatile hydroxide. By reducing the thickness of the chromine layer and by accelerating the oxidation kinetics that this induces, the end of life of the alloy is then precipitated.

It is therefore essential to better understand the oxidation kinetics and degradation mechanisms of metal alloys, as well as the influence of the evolution of the gas phase on the oxidation and volatilization kinetics, and on the degradation mechanisms of alloys subjected to such environments.

The proposed Master's internship will take place at the LGC, as part of the ANR DYNAMIC project which brings together 3 CNRS laboratories (the CIRIMAT, the LGC and the IJL) and 2 industrial laboratories (Air Liquide and Safran) around the sustainability of metallic materials regarding high-temperature corrosion under oxidizing conditions in the presence of water vapor, representative of current and future industrial processes.

As part of this project, through a PhD thesis (G. Duthoit, defense scheduled for early 2026) and a Master's internship (A. Faye, Feb-July 2025), high temperature oxidation tests were conducted at CIRIMAT, in parallel with numerical simulations of the gas phase within the oxidation bench performed at the LGC by CFD (Computational Fluid Dynamics). Thus, it was possible to quantify the impact of the enrichment of the gas phase into volatile species on the volatilization kinetics of several samples placed in series [1-2]. The results obtained are original compared to the state of the art, but they only concern a single oxide (Cr_2O_3), a single volatile species ($CrO_2(OH)_2$) and only simple sample geometries, far from the complex geometries of interest in aeronautics.

The objectives of the internship are to:

Conduct a bibliographical study on subjects of interest for the study,

- Take in hand the CFD calculation model Fluent Ansys ® already operational,
- Simulate the appearance of other oxides (e.g. rich in Ni, Ti and/or Nb) and their volatilization,
- Analyze the impact of increasing the specific surface area of the oxide layer on the phenomenon of volatilization,
- Simulate sample geometries close to those of aircraft turbine blades, and compare the results of the calculations with those that will be obtained experimentally as part of another Master's internship.

The internship will be co-supervised by the LGC (H. Vergnes and B. Caussat, CVD team, IRPI department, Engineering of Innovative Polyphase Reactors), and the CIRIMAT (A. Vande Put and D. Monceau, MEMO team, Mechanics, Microstructure, Oxidation and Corrosion).

Start of the internship: February or March 2026
Duration of the internship: 5 to 6 months
Location : LGC-ENSIACET in collaboration with CIRIMAT-ENSIACET, Toulouse
Application deadline : End of November 2025

Candidate profile: Skills in process engineering, chemical engineering or materials engineering, with if possible knowledge and/or first experience in numerical simulation by CFD

Application to be sent to:
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References :

- [1] Influence of water vapor rich environment and gas velocity on the oxidation kinetics of in625 at 900°C: experimental study and CFD gas phase simulation, G. Duthoit, H. Vergnes, D. Monceau, B. Caussat, A. Vande Put, *High Temperature Corrosion of Materials*, Vol. 101, 1513-1526 (2024). https://doi.org/10.1007/s11085-024-10307-1

- [2] Expériences et simulation CFD : un couplage pertinent pour comprendre l'influence de paramètres clés sur la volatilisation d'un alliage chromino-formeur exposé à un environnement humide, G. Duthoit, A. Vande Put, B. Caussat, H. Vergnes, D. Monceau, Congrès *La métallurgie, quel avenir !* (Juin 2025, Toulouse).